

HANDBOOK FOR THE
CHEMICAL
ANALYSIS
OF PLASTIC
AND
POLYMER
ADDITIVES

SECOND EDITION

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inappropriate ingredients were identified in the raw materials. Analysis and identification of non-disclosed ingredients was often hampered by application of proprietary materials that may have been suitable for one application, but unacceptable for another.

Mr. Groeger has developed new materials for medical delivery devices, battery seals and insulators, electrical insulation systems, flame-retardant materials, coatings, food packaging, adhesives, and others. He is president of Mantis Associates, Inc., which is dedicated to product development in consumer products, food packaging, and drug delivery devices/systems, among others. Mantis also specializes in materials development and applications, failure analysis, and selected areas of litigation support. Mr. Groeger has published extensively and presented at international conferences and various universities. He is an active member of the American Chemical Society, Society of Plastics Engineers, Institute of Electrical and Electronics Engineers (IEEE), and holds numerous patents that focus on polymer applications. He has served a consulting role to various federal regulatory and state law enforcement agencies in addition to serving a wide range of industrial clients.

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Importance of Polymers

Polymers touch virtually all aspects of our lives, from everyday packaging to unseen applications such as gas pipelines under our streets. Polymers can include simple thermoplastics like polyethylene, a huge range of rubber compounds, adhesives, coatings, sealants, and many others. We wear polymers, we walk over them, we are fed with them, we coat our metals with protective polymers, and we even use polymers in the preparation of materials such as ceramics. Polymers are typically identified on the basis of the principle polymeric component. Terms like polypropylene, polyvinylidene fluoride, polycarbonate, and ethylene-propylene rubber identify a base polymer; however, these are seldom used in pure form for a number of reasons that underlie the basis for this reference handbook. The wide-ranging usefulness and applications of polymers result from the ability to modify the base polymer through the use of organic and inorganic additives. Additives can be used to tune a polymer to a specific application, imparting high temperature oxidation resistance, improved flexibility, color retention, anti-static performance, or adding impact resistance. Other polymers are compounded for economic reasons, where a costly base polymer may be extended by addition of lower cost additives such as clays, reground polymer, other polymers, or a blowing agent that reduces density. There are a number of established reference handbooks that address the selection and application of performance-enhancing additives for polymers. Polymers compounded on a commercial scale are described in catalogs or product data sheets that list the performance properties, typical applications, and a general description, but formulation details typically remain proprietary.

Formulation: Choosing an Application-Specific Polymer

Unlike foods and personal care products, manufacturers of polymers are not required to disclose the ingredients that have been incorporated into their compounds. Polymer compounding information is typically proprietary, with types and concentrations of ingredients carefully protected as intellectual property. Formulation information provided through Material Safety Data Sheet (MSDS) disclosure is typically incomplete or non-specific regarding the identity of all of the ingredients. Instead, many components are only identified during troubleshooting or product review. The polymer supply chain is complex and intermediate suppliers may not have any direct knowledge of the end use for their materials. For example, cross-linked rubber articles must cure quickly in the mold to assure a commercially profitable throughput. This may require excess curing agent and a synergist, both of which leave potentially undesirable extractable compounds in the final product. Injection molded plastic components are typically unit-priced, again making high mold throughput essential. This encourages the use of melt flow modifiers, internal lubricants, and external lubricants that act as mold release agents. If the compounder purchases a base polymer from a multi-market supplier, but is making the choice on the basis of a generalized description or processing properties, the end product may be inappropriate for the application.

Through many years of analyzing polymers for a wide range of applications, we have worked extensively within the polymer supply chain in areas that include troubleshooting and developing compounds for specific applications or process improvement. It is our hope that this practical experience combined with the proper analytical technique will provide a solid basis for informed decision making and awareness of the complexity of polymeric materials and their compounding.

Additives as Possible Hazards: Extractable and Leachable Compounds

Additives can be candidates for both extractable and leachable compounds. Extractable compounds are released from the plastic/polymer matrix through solvent-based techniques or thermal desorption — see Table 1 in Chapter 2, Extraction and Analysis. Leachable compounds are removed from the polymer by interaction(s) with the contents of the package. The composition of the package contents controls the leaching process based on solubility and diffusion. Leachable materials will be removed to various levels based on the presence of water, oils, salts, and other organic compounds. Additional considerations include pH and temperature. Besides additives, extractable and leachable entities may include breakdown products of the base polymer as well as the primary formulation ingredients and their breakdown products. Both types of compounds are a major concern for the pharmaceutical and food packaging industries. Case studies illustrating examples of extractable and leachable contaminants appear in another section of this book.

Increased attention also has been directed to some of the higher volume organic additives in polymer compounds such as plasticizers, flame-retardants, and antioxidants. Ongoing studies have shown that some of these compounds are human health hazards and include endocrine mimickers, endocrine disruptors, suspected carcinogens, or pathogens. Ingredients that have been used for many years are now being scrutinized when they may have been overlooked in the past for lack of reference information and/or suitable reference compounds. Some states such as California are taking additional steps to regulate these chemicals in consumer goods leading to the recently proposed ban on phthalates and bisphenol-A in children's items, for example. Some of these compounds are regulated through government agencies such as the US Food and Drug Administration (FDA), and guidelines are available through the US Code of Federal Regulations (CFR) for use in consumer applications. Compared to regulations for other items, however, plastics and polymers are surprisingly unregulated for most uses. This is in the process of changing as consumer concern and government regulations will force manufacturers of toys, food packaging, pharmaceutical packaging, and even wire and cable to be held accountable for the materials they use.

Importance of Analysis

Identifying materials in the final plastic/polymer by analysis is extremely challenging. Although many reference handbooks exist that address the selection and application of performance-enhancing additives and formulation ingredients for polymers, there really is no comprehensive reference for the identification of these compounds in raw materials or finished goods. This handbook aims to fill this void by providing a comprehensive reference library for chemists; and to provide the information needed to extract, identify, and quantify additives used in polymers and plastics by a common, readily available laboratory technique — gas chromatography/mass spectrometry (GC/MS).

The analysis of these materials is even more critical with increased interest in their environmental impact on ecological systems and human health. A number of frequently used additives, such as phthalate and adipate plasticizers have been identified as environmental pollutants, and the fate of these chemicals is the subject of ongoing studies. Concern over the total composition of plastics has increased the focus on the total life cycle of polymeric materials. Government attention to toxic substances has increased over the years through the US Toxic Substances Control Act (TSCA) and the REACH initiative in the EU. These regulations may prohibit or otherwise impact the exportability of the plastic goods or other products that come in contact with the plastics. This, coupled with increased consumer attention and disclosures of “chemicals” in consumer products, has increased the need for a more complete analysis of polymeric materials. Combustion of rubber

and plastic materials for energy production has also increased the awareness of organic and inorganic additives and the analysis of these products. Unintended combustion in fires, for example, has led to a significant increase in sensitivity to desorbed organic compounds and decomposition products in closed environments. This application has greatly affected the formulation of polymeric materials used in aircraft furnishings and building wiring.

Analytical Protocols, Historical

During our years of performing analyses of polymers, many of the commercial materials were found to contain ingredients that made little intuitive sense when considering the final application. In many cases, polymers were submitted for analysis due to poor or inconsistent performance, unusual interactions with other components in a device, or even release of compounds into a food product, pharmaceutical compound, or implantable medical device. Based on this data, it was obvious that comprehensive protocols for the analysis of plastics/polymers needed to be developed. In the past, analytical protocols included extractions performed with a polar and a non-polar solvent used to extract organic compounds from a polymer for subsequent analysis by GC using a flame ionization detector (FID). FID alone may not be a definitive test, since the identity is based on column retention time, which is not a unique characteristic for identifying many of these complex organic compounds.

It is our practice to analyze polymers primarily through thermal desorption and GC/MS. Solvent extraction is used for comparison purposes when necessary. Typically, our approach has been to analyze for all volatile compounds present in a polymer, even those that are inappropriate for the application under review. While not always the case, many analyses have provided insight that led us into developing application-specific polymer compounds through direct interaction with the supply industry.

Purpose

The primary aim of this Handbook is to provide the tools to help a bench chemist obtain a more complete listing of additives present in a particular polymeric matrix. It is designed to serve as a reference for the chemist who is monitoring a polymer/plastic material for regulatory or internal compliance. The techniques that we have been using successfully are described in this book to help the analyst to correctly identify the complex nature of the materials that have been added to the polymer/plastic. We provide information on analyzing polymers through thermal desorption, and the use of GC with a mass selective detector (MSD). Many compounds break apart either during extraction or analysis, so identification by key fragments, and typical moieties for the final compound is critical. The use of the GC/MS system allows the analyst to characterize a compound based on the utilization of these fragments or moieties.

To add even more complexity to an already daunting challenge, many additives are disclosed by trade name, not chemical name or CAS number. This Handbook aims to address all of these considerations by providing a listing that can be cross-referenced by trade name, chemical name, CAS number, and even key mass unit ions from the GC/MS run. This Handbook serves as a library of additives that can be used to identify compounds commonly found in polymers/plastics.

Polymers have undoubtedly changed the world and have provided countless products that directly affect our quality of life. Proper development and use of plastics/polymers remains a paramount responsibility. As more regulations are promulgated, and with the continued oversight of possible health hazards presented by the additives incorporated into these materials, it becomes imperative

that the monitoring of these compounds is supported by high-quality reference materials and dependable analytical techniques.

HOW TO USE THIS HANDBOOK

The information presented in this Handbook was formatted in a consistent manner to provide a useful resource for a chemist performing practical or investigative analyses. Compounds were selected to obtain a representative sampling of the primary classes of polymer additives.

For each material or compound listed in this Handbook, the following information is presented:

The Data Section:

- *Chemical Information.* Information in this section includes the unique structure (if available), CAS and Registry of Toxic Effects of Chemical Substances (RTECS) number (if available), common abbreviations (if available), chemical formula, and molecular weight.
- *Trade Names and Manufacturers.* Many of these organic materials are produced under a variety of trade names. This section lists other manufacturers that may produce the same compound under a different trade name. The corresponding names are all cross-referenced in the Subject Index.
- *Physical Properties.* This section contains the general physical properties of the compound. For the solubilities, the following abbreviations are used: U — Unknown, S — soluble (solvent identified), P — partially soluble (solvent defined).
- *Application, Regulatory, and Environmental Information.* Information regarding the applications and regulations concerning the compound are contained in this section. Laws and regulations, as well as our understanding of the toxicity and nature of chemicals, change on an ongoing basis. Please use this text as a reference while independently determining the present status of any regulations prior to proceeding with any project.

The Mass Spectral Information

This section includes the actual GC/MS analysis of the compound. This may contain from one to three pages of data, depending on the nature of the material. Tabulated for each spectrum is the mass-to-charge ratio of the five most abundant ions in the spectrum, as well as the molecular weight of the material.

The Appendices and Indices presented in the later sections of this Handbook are described as follows:

Appendix A

This section contains chromatograms for all the compounds and the corresponding analysis conditions.

Appendix B

This section contains a list of definitions and abbreviations used in the Handbook.

Subject Index

In addition to key words and terms, this index contains the synonyms listed in the text, cross-referenced to the corresponding pages.

Five Peak Index

This index can be used to identify an unknown compound from your own analytical data. This contains the following data, tabulated by the 100% abundance ion from each mass spectrum:

- The first five columns include the mass-to-charge ratios of the five most abundant ions in the spectrum — with the most abundant noted in bold.
- The MW column presents the molecular weight of the parent compound as reported in the text.
- The relative intensities of the five most abundant ions (integral values, proportional to 100 for the most abundant ion).
- The compound name and corresponding page number of the compound of interest.

*Molecular Weight Index**CAS Number Index**RTECS Number Index*

Overview of Polymers, Additives, and Processing

Introduction

Polymers are available in a wide range of formulations and properties achieved through selection of the base polymer and additives. Two types of chemical reactions produce polymers:

- 1) Condensation between polyfunctional molecules (monomers) that react with each other. This reaction is heat driven, sometimes with the aid of a catalyst. The longer the exposure to heat, the longer the polymer chain becomes. A common example of this is nylon, a reaction of a diamine with a dicarboxylic acid producing a polyamide.
- 2) Reaction of a molecule that is activated with an initiator to form a free radical. This free radical, when reacting with a “normal” molecule creates a new free radical, causing a full fledged chain reaction. This process creates, from a monomer, a long chain polymer instantaneously. No intermediate chain length polymers are present. This process is also called vinyl polymerization.

Most polymers are identified on the basis of their common name. Examples include polyethylene, polyvinyl chloride, butyl rubber, acrylonitrile-butadiene, and styrene (co-polymer ABS). However, few polymers are used in pure form since they often require chemical modification to achieve optimum properties and promote non-inherent performance. Some of these property enhancements include improved resistance to oxidation, high temperatures, flammability, impact loads, surfactants, ultraviolet radiation, as well as modification of a wide range of other properties. The process of adding essential ingredients to polymers to achieve these results is termed compounding. However, it is generally not practical to precisely match the inherent properties of a base polymer to a specific application. While some polymers such as polyethylene are available with a wide range of properties based on a range of molecular weights, molecular weight distributions, and tacticity (stereostructure), other polymers have a finite range of properties for which compounding provides a practical method for adjustment of general or specific properties. For example, polyvinyl chloride is the most commonly used thermoplastic. In the raw form, this is a rigid, transparent polymer; however, in the most familiar applications, this “vinyl” polymer is flexible and colored as in black electrical tape or a yellow rain coat.

As stated above, the modification to achieve these results is usually achieved by mixing a polymer with other polymers, both organic and inorganic materials including additives, metal powders, glass fibers, and other materials to match the end-use application.

This chapter addresses three basic classes of polymers and the approaches for processing them into practical compounds. These classes include thermoplastic polymers, and two types of elastomers — crosslinked elastomers and thermoplastic elastomers. Compounds prepared from each class have a range of achievable properties, and each category of compounds may have overlapping properties. Each category is prepared by different technical approaches with varying controls, energy requirements, and limitations. A brief definition of each class follows. Also included, later in the chapter, is a detailed description of how additives influence the production process. The overview of polymer compounding is presented next to provide the analyst an introduction into the many processing steps where polymer composition changes occur, deliberately and otherwise.

Classes of Polymeric Compounds

In the form of raw materials, polymers exhibit a wide range of compositions and properties. These properties can be enhanced or tuned to specific applications through the preparation of compounds. This section addresses three basic classes of polymers and the approaches for the preparation of compounds.

Thermoplastic Polymers

Thermoplastics are polymers that can be melted, prepared into a desired form, and then re-melted. Thermoplastics can be processed into a desired shape through many processes, the most common of which are injection molding and extrusion. Blow molding, transfer molding, calendaring, casting, and other forming operations are all possible with thermoplastics.

Crosslinked Elastomers

Crosslinked elastomers are polymers that are first prepared by compounding a base elastomeric polymer with property-modifying additives and a reactive crosslinking agent. Polymers of this type can be formed into a desired shape through many different operations; however, the final operation requires that the shaped article be heated to a temperature at which the crosslinking agent decomposes to produce free radicals. These radicals react with the base polymer to form chemical crosslinks transforming the linear “two-dimensional chain” into a “three-dimensional object”. This class of material cannot be melted and reformed. Alternate crosslinking methods are used for special applications including the use of ionizing (gamma) radiation, ultraviolet radiation, and water-initiated (silanol) cure systems.

Thermoplastic elastomers

Thermoplastic elastomers (TPEs) are a more recently developed class of polymer in which the neat polymer has inherently elastomeric properties, yet it behaves thermoplastically. With some limitations, these materials can be formed by essentially the same operations as thermoplastics, but the final object exhibits elastomeric behavior. Objects molded with thermoplastic elastomers can be melted and re-shaped. Since these are not crosslinked, their creep resistance and extended high temperature use are limited.

Thermosets

This family of polymeric materials includes liquid polymers and thermoplastics that have been crosslinked. Preparation of thermosets follows the same compounding route used for thermoplastics; however, a crosslinking agent or ionizing radiation are used to form chemical crosslinks.

Liquid polymers can be chemically crosslinked to form thermosets. Materials in this category include epoxies, embedding compounds, coating materials, urethanes, silicone polymers, and others. Due to the inherently low viscosity of liquid polymers, they are compounded using a variety of mixing systems, including high shear devices.

Compounding Objectives

Polymeric compounds must behave as a *system*, consisting of the base polymer and additives, selected to achieve a set of final properties. During compounding, mixing must occur at two fundamental levels — dispersive mixing and distributive mixing. *Dispersive mixing* relies on shear action to blend the additives into the polymer. Dispersive mixing must overcome differences in viscosity, surface energy, chemical compatibility, melting temperature, and others to achieve

overall homogeneity of the formulation. Improperly dispersed polymer compounds will typically contain domains where ingredients have not been blended properly, as shown in Figure 1-1. Dispersive mixing focuses on short-range blending of the compound, while distributive mixing addresses the overall homogeneity of a batch. *Distributive mixing* places different requirements on the mixing process, depending on the type of equipment that is being used. This will be further addressed in the [Compounding Overview](#) section in this chapter.

During the compounding process, it is essential that all ingredients added to a polymer are retained within the compound in a stable manner that assures functionality. Thermal degradation and excessive shear action may selectively degrade different additives. It is imperative that processes are developed and validated by functional testing of the final compound. Mixing processes must be very carefully controlled to assure consistent quality. Variations in compound quality can have an adverse and varying impact on components prepared from the compound.

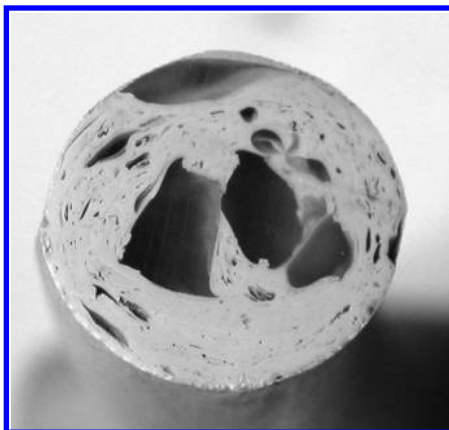


Figure 1-1 Example of Poorly Mixed Polymer Compound

Thermoplastic Compounding

Thermoplastic compounds are typically prepared by mixing organic or inorganic compounds with a single base polymer, copolymers, or blends. The base polymer may consist of a chemically bonded blend such as the block copolymer acrylonitrile-butadiene styrene (ABS) or a second base polymer may be used to enhance the overall end properties of the compound.

A base polymer, such as an ethylene-propylene (EP) copolymer, can be acquired in a range of compositions, molecular weights, various ethylene-to-propylene ratios, various molecular weight distributions, and a range of densities. Each of these variations results in a base polymer that has specific practical properties such as flexibility, elastic recovery, tensile strength, and thermal limit to name a few. As a base polymer, ethylene-propylene polymers and most other non-crosslinked elastomers have no significant commercial application, since they are essentially a liquid with very high viscosity.

Organic Additives

Antioxidants

Thermoplastics may contain a wide range of organic additives that are incorporated into the polymers to improve selected properties. In virtually all cases, an antioxidant must be added to allow the compound to be blended with other ingredients, to be pelletized or chopped into

intermediate form, and to survive thermal stresses associated with the final forming process. In some cases, the base polymer is blended with an antioxidant at the time of preparation of the base resin. This type of antioxidant is intended to add thermal stability for processing considerations. External antioxidants can also be added to improve shelf life of the product or to improve its high temperature stability, while adding a stability margin during thermal processing.

Internal Lubricants

These may be added to the polymer to reduce the shear rate during processing, especially when an inorganic material is being added. If the shear level gets too high, thermal damage and polymer chain scission can result. The lubricant must be selected properly to avoid having it decompose or affect the polymer compound in some adverse manner. Common lubricants include fatty alcohols (C14-C18), fatty acid esters (C14-C18), dicarboxylic acid esters (C14-C18), fatty acid amides (C16-C18), and esters (C26-C32).

Release Agents

They are often blended into compounds that are developed for injection molding applications. Where such an additive is absent, molded components tend to stick to mold surfaces. To prevent this, mold surfaces must be treated between every cycle, or they can be coated with a range of semi-permanent mold release treatments. Inclusion of an internal release agent prevents mold surface build-up, surface charring, and simplifies production. Internal mold release agents may include hydrocarbons, alcohols, carboxylic acids, halogenated compounds, ketones, carboxylic acid esters, amides, metal salts, and silicone compounds.

Plasticizers

Plasticizers are added to thermoplastic compounds to improve flexibility, increase the acceptance level for inorganic additives, and to aid in processing, such as melt flow reduction. Synergistic effects can also be obtained such as reduction of shear during mixing and improved impact resistance. Plasticizer compounds typically include phthalates, adipates, esters, and fatty acid esters (oleates, palmitates, stearates).

Impact Modifiers

These are often added to otherwise brittle thermoplastics to improve impact resistance. In some cases, the addition of inorganic materials renders plastics hard and brittle, thus requiring the addition of an impact modifier. Impact resistance can be improved through addition of polymers with increased flexibility or elastomeric characteristics. Acrylics and butadiene are common impact modifiers. Styrene is commonly impact-modified through graft polymerization with acrylonitrile or polybutadiene (hence ABS [acrylonitrile-butadiene-styrene]), or it can be grafted to an ethylene propylene diene elastomer. Polypropylene can be made impact resistant through various blending methods to incorporate ethylene-propylene monomer.

Electrostatic Control Agents

They are required for thermoplastics applications where surface electric charge must be controlled or prevented. There are a number of compounds available for this function and these can be divided into two general categories: bulk and surface-modifying. Bulk additives may be simple, such as carbon black, which, when added in sufficient concentration, provides a semiconducting matrix, thus controlling the accumulation of localized charge. Metal salts can also be used for this purpose in some polymers. Cationic compounds can impart bulk conductive properties and these include compounds with a bulky cation such as quaternary ammonium, sulphonium salts, or imidazoline compounds. Anionic compounds are also used and these include, for example,

alkylsulphonates. Nonionic compounds can also be used for controlling charge distribution through interfacial activity. Compounds in this category include ethoxylated fatty amines, ethanolamides, polyethylene glycol esters, and others. Some organic compounds are also useful for controlling surface charge. These function by having limited solubility in the host polymer. Compounds of this type migrate to the surface of the polymer where their nominally low concentration increases locally at the surface, and thus provide a conductive surface bridge.

Dyes and Organic Pigments

Dyes are chemical compounds that impart color to plastic compounds. These dissolve in the host polymer and are therefore not present as discrete particles. Dyes are typically azo or anthraquinone compounds.

Pigments are discrete particulate materials of very small particle size, which are blended into a thermoplastic compound to impart color. Organic pigments are typically of an azo or cyanine structure. Most organic pigments also have good thermal stability across the thermoplastic processing range; however, they are less well-suited for crosslinking and elevated temperature applications. Due to their insolubility in the polymer, these serve as nucleating agents during recrystallization. Thus, pigments may play a significant role in controlling the final properties of a compound.

Polymer Blending

For some applications, polymers are blended to provide a balance of properties. Some polymers blend well due to mutual solubility, but if the solubility parameter of the candidate polymers is different by more than about 3 SI units, the polymers must be blended with an intermediate material to improve compatibility. Typically, this involves an intermediate polymer with a low molecular weight. In the melt, this serves to reduce the surface tension between two incompatible polymers, thus improving dispersion. Low molecular weight polyethylene is an example of a polymer blending aid. In other cases, metal stearates or salts can be used to aid dispersion. Examples include zinc stearate and calcium stearate.

Inorganic Additives

Fillers and Reinforcers

Thermoplastics often have physical properties that are inherently well suited to a particular application. In such a case, there is little need for addition of inorganic materials. Inorganic additives are very useful for improving the physical strength and deformation resistance of thermoplastics. They function by forming a network of pinning points in the polymer wherein the slippage of polymer chains under mechanical stress is impeded. Inorganic reinforcements are of many types, ranging from natural minerals to synthetic minerals to specialized materials with directional physical properties. Clays in common use for higher quality plastics include kaolin, other natural silicates, and others. Synthetic and high purity reinforcements include titanium dioxide, calcium carbonate, silica, and many others.

Inorganic additives are also useful for controlling the onset temperature, extent, and dimensions of the crystalline phase in semi-crystalline polymers. The inorganic component acts as a site for heterogeneous nucleation of polymer crystallites. By initiating nucleation at many closely spaced sites, the polymer solidifies with a network of small uniformly distributed crystalline domains. By balancing the comparative strengths, flexibility, and creep resistance of crystalline and amorphous phases of a polymer, a balance can be achieved for engineering applications. Heterogeneous nucleation is also helpful for controlling the structure of polymers with a slow rate of

recrystallization. During injection molding, for example, as the molded part cools, heat transfer to the chilled mold causes the polymer in the outer surface of the part to nucleate first, followed by the core of the component. Heterogeneous nucleation occurs at the mold interface, but homogeneous nucleation may occur in the core of the sample. This would proceed slowly due to the ratio of heat capacity of the polymer to poor thermal conductivity. Addition of a matrix of fine inorganic particles increases molding throughput and improves the bulk properties of the polymer. Titanium dioxide and silica are typical additives in this category. Titanium dioxide has a dual purpose in many cases in that it is a very efficient whitener. Nucleating agents can also have the form of dispersed polymers with a higher melting point.

Inorganic Pigments

Wide ranges of compositions are used to impart color to thermoplastic compounds. Pigments are discrete particulate materials, of very small particle size, that are blended into a thermoplastic compound to impart color. Inorganic pigments are commonly found in the form of metallic compounds. Oxides of iron, chromium, molybdenum, cadmium, nickel, antimony, and titanium produce a wide range of vivid colors. Variations in oxygen stoichiometry have a pronounced effect on the color of many of these metal oxides. Carbon black is also a very effective colorant. Inorganic pigments are very stable in a polymer and generally exhibit high color retention. These often have a synergistic effect on the recrystallization performance of polymers during thermal processing, due to their role as heterogeneous nucleation sites.

Crosslinked Elastomer Compounding

Organic Additives

Antioxidants

Raw elastomeric polymers typically contain an antioxidant that is added at the time of manufacture to provide thermal stability for compounding, milling, and subsequent operations to produce beads, bales, or other forms where the polymer is first heated, then cooled into an intermediate form for storage, transport, and metering. The as-provided antioxidant does not generally provide sufficient stability to protect an elastomeric compound through final forming and curing due to the high shear energy required for mixing. External antioxidants are often added to provide additional protection. Antioxidants are available in many forms and they vary in functionality, according to their composition and structure. Typical antioxidants for elastomers include a range of phenolics, amines, and bisphenol derivatives.

Crosslinking Agents

Elastomers must be crosslinked to hold their final form. The crosslinking reaction takes place through generation of free radicals that promote bonding at sites of unsaturation. The most common crosslinking agents for this include reactive peroxides, such as dicumyl peroxide, diacetyl peroxide, di-tert butyl peroxide, and others. Since each has a different temperature at which thermal decomposition initiates, curing conditions vary with the peroxide type.

For some products, elemental sulfur or sulfur-containing benzothiazole compounds are added to the compound as a curing agent. Sulfur reacts to form C-S-C bonds. This is an inexpensive reaction scheme and it is useful for production of rubber compounds across a very wide hardness range. Residual sulfur compounds lead to odors and acid products that are not well suited to applications where clean materials are desired. Thiazole compounds provide better handling and more controllable crosslinking processes, with low residual odor and extractables.

Cure Rate Modifiers

The crosslinking reaction rate may be too slow for some commercial processes and the reaction may exceed the oxidation resistance time for the elastomer compound. In such cases, curing accelerators are used with the sulfur-curing process. Zinc oxide is a commonly used accelerator; however, thioureas, hexamethylenetetramine, and others are effective. For organic peroxides, the cure rate can be greatly increased with an increase in applied temperature, though oxides of zinc, magnesium, or calcium can be used to limited effect. The rate of crosslinking reaction can be slowed for those cases when the rate exceeds the formation process for some components. Cure retarders include compounds such as nitrosodiphenylamine, benzoic acid, and phthalic anhydride. Use of a cure retarder increases the burden on an antioxidant to protect the polymer against thermal degradation.

Lubricants and Related Compounds

During the compounding operation, shear stresses in an elastomer compound are very high. To reduce shear and to promote more efficient wetting of inorganic ingredients, processing aids can be used. Zinc and calcium soap compounds are very efficient for reducing shear viscosity during mixing. Fatty acid compounds and fatty acid esters are also useful and examples include stearic acid and palmitic acid. Various hydrocarbon oils are often used for shear viscosity reduction. These may include high purity white mineral oils.

Coupling Agents

Elastomer compounds are typically blended with an inorganic reinforcement to provide enhanced physical properties. Bonding between these is typically mechanical rather than chemical in nature. Due to the high flexibility of elastomers in normal applications, shear stresses at the interface between the inorganic and polymer can cause a failure of the mechanical bond. For high performance compounds, a coupling agent is used to form a chemical bond between the host polymer and an inorganic, such as kaolin clay. Typically, siloxane compounds are used as coupling agents.

Carbon Black

Carbon black is a very effective strength modifier for a wide range of elastomeric compounds. Since carbon black contains reactive surface groups, it bonds and interacts efficiently with the base polymer. Carbon black can be blended from a concentration of a few phr (parts per hundred resin by weight) to as much as 40 phr to achieve a wide range of physical properties. Due to the chemical bonding between carbon black and rubber, it is very effective at increasing hardness without a corresponding major reduction in tensile strength, tear resistance, or elongation limit. Carbon black addition reduces the free volume in rubber compounds, thus improving solvent tolerance, oil tolerance, and gas impermeability. Carbon black improves oxidative stability and protects the polymer against UV damage. Carbon blacks are available from a range of sources and all are produced from an incomplete combustion process. Sources include oils, tars, and reclaimed hydrocarbon materials. In other cases, carbon blacks of high purity can be derived from acetylene gas, low molecular weight polymers, and other clean sources.

Release Agents

Organic release agents and anti-blocking agents are occasionally used for elastomer compounds. Generally, these compounds have limited solubility in the elastomer compound, so they migrate and concentrate at the surface, where they can be effective to prevent cohesion and/or adhesion. Waxes and high molecular weight adipic acid esters are examples of compounds in this category.

Liquid polymers are occasionally used for softer grades of rubber compounds, where a base polymer will not provide the required balance between strength and flexibility. Liquid rubbers are of low molecular weight and would be fairly useless unless blended with other materials. In some cases, an external diene is added through a liquid base polymer. Liquid rubber is typically added during the milling operation.

Plasticizers

Elastomer compounds can be plasticized by addition of organic compounds. Elastomer compounds are inherently flexible and selection of a base polymer on the basis of molecular weight characteristics, chemical composition, and degree of crystallinity serves as the basis for the properties of the compound from which an elastomer is made. Oils are the most common plasticizer for elastomers. Oils of paraffinic structure or aromatic structure can be used with elastomers in which they are compatible. Paraffin wax would also be included in this category. Other plasticizers include phthalic acid esters and adipic acid esters. Fatty acids can be used as plasticizers but these contribute to an increase in surface tack of elastomer compounds. Examples include stearic and palmitic acid. Plasticizer addition has the added benefit of aiding with incorporation of inorganic materials.

Pigments and Dyes

Color-tinting of crosslinked rubbers follows the same description presented for thermoplastic compounds. A major problem with the use of organic pigments and dyes is that many decompose when high temperature curing agents are used. For these compounds, inorganic pigments are typically the only option.

Inorganic Additives

Fillers and Reinforcement Agents

Many commercial elastomer compounds are mechanically reinforced through the addition of inorganic compounds. These physically and/or chemically bond to the polymer to provide a more rigid matrix. Reinforcement agents include talc, various clays, silica, titanium dioxide, and many others. In some cases, fillers with high aspect ratios are used to impart directional reinforcement. A balance between particle size, surface structure, and dispersion efficiency is necessary for obtaining the best and most uniform performance of an elastomer compound. Many inorganic additives are first dried at high temperature (calcining) to split off water of hydration. This prevents moisture release during compounding and crosslinking. Moisture produces voids and often inhibits proper curing of crosslinked elastomers.

Inorganic additives for rubber compounds also include materials that enhance performance under various accelerated stress conditions. Zinc oxide is an effective heat stabilizer for some types of elastomers. Iron oxide, lead compounds, barium salts, and specially treated clays, such as kaolinite, add performance margin in wet service conditions.

Thermoplastic Elastomer Compounding

Compounded polymers prepared with thermoplastic elastomers (TPE) are prepared in much the same manner as thermoplastics, with some exceptions. Thermoplastic elastomers generally combine the flexibility and frictional behavior of rubber compounds with the practical forming considerations of thermoplastic materials. These are commonly encountered in automotive and appliance applications where non-slip surfaces are desirable. Since compounds in this class have elastomeric physical characteristics, this often requires that a twin-screw mixer makes use of

screws with a profile that is different than for thermoplastic compounding. Differences include the use of tapered screws, an increased frequency of barriers along the screw length to increase localized shear, separate zones of high and low shear action, and others. TPE compounds use mixers with high length-to-diameter (L/D) ratios (see [Compounding Overview](#) at the end of the chapter).

Thermoplastic elastomers are most commonly formulated from elastomeric polyurethane or block copolymers of polystyrene-elastomer, polyamide-elastomer, or polyether-elastomer bases. Thermoplastic elastomers are provided as a raw material in pelletized form for subsequent compounding. The internal domain structure that is required for thermoplastic-elastomeric performance has been established by specific considerations of blending and structural-chemical interactions. In compounding operations, specific temperature ranges are required to assure that phase separation does not occur in the TPE base polymer.

Organic and inorganic compounds for modification of thermoplastic elastomers follow the previous descriptions for thermoplastics. Addition of inorganic materials requires a screw type mixer with sufficient cooling to remove the heat developed due to high shear viscosity. The mixer must also include some areas with very high shear to assure proper dispersive mixing. Antioxidants for thermoplastic elastomer protection during compounding must have good longevity at elevated temperature and they must have good solubility in the compound to prevent separation.

COMPOUNDING OVERVIEW

Introduction

This overview of polymer compounding was prepared to provide the reader with an overview of compounding methods and equipment. Since possible contamination and subsequent failure of an end product can be associated with a compounding process, the authors believe that a brief introduction into the engineering and practical aspects of compounding is relevant.

Methods of Compounding: Thermoplastic Polymers

Thermoplastic polymer compounds are typically prepared by use of a single- or twin-screw mixer. This consists of parallel, threaded cylinders (screws) that are enclosed within a heated barrel. Heating is applied and separately controlled in zones along the barrel. The screws are caused to rotate with a gear reduction electric drive at one end. The barrel is a high strength enclosure, designed to sustain very high pressure, temperature, and shear conditions. The screws counter-rotate and the rate is variable. At the driven end of the mixer, polymer is added through a hopper into the throat of the mixer. Pre-weighed and mixed additives are also incorporated or metering hoppers may add proportioned quantities of polymer and additives that will form the compound. Due to the threaded nature of the screws and their proximity in an enclosed heated barrel, the ingredients are subjected to high shear as they melt. The thread pitch causes the compound to travel down the barrel, where mixing time increases and viscosity drops as the compound heats. Mixers for thermoplastics typically have long barrels and a length-to-diameter ratio of at least 20. At the end of the mixer is a screen pack, followed by a die for extruding the compound into tapes, strands, or other forms. A rotary cutter may be mounted over a strand die to produce the “pellet” form in which the bulk of thermoplastics are supplied. The screen pack is used to remove any non-dispersed materials and to capture large particles or contaminants that would otherwise be detrimental to the finished compound. The screen pack also contributes to effective mixing by providing back pressure.

Figure 1-2 presents an illustration of several types of mixing screws. These show variations in thread pitch as different profiles or offsets in the diameter of the screws between the threaded lands. Screw profiles vary for the type of compound being mixed. In some cases, very high shear is required to assure proper dispersion of ingredients. For other compounds, aggressive shear will damage the base polymer, so reduced shear and longer mixing times are targeted. Screw profiles vary in thread land, length, and distribution of thread pitch along the screw length. Some screws contain radial pins, staggered knives, or other features for specialized applications. Some mixers include three or more nested screws.

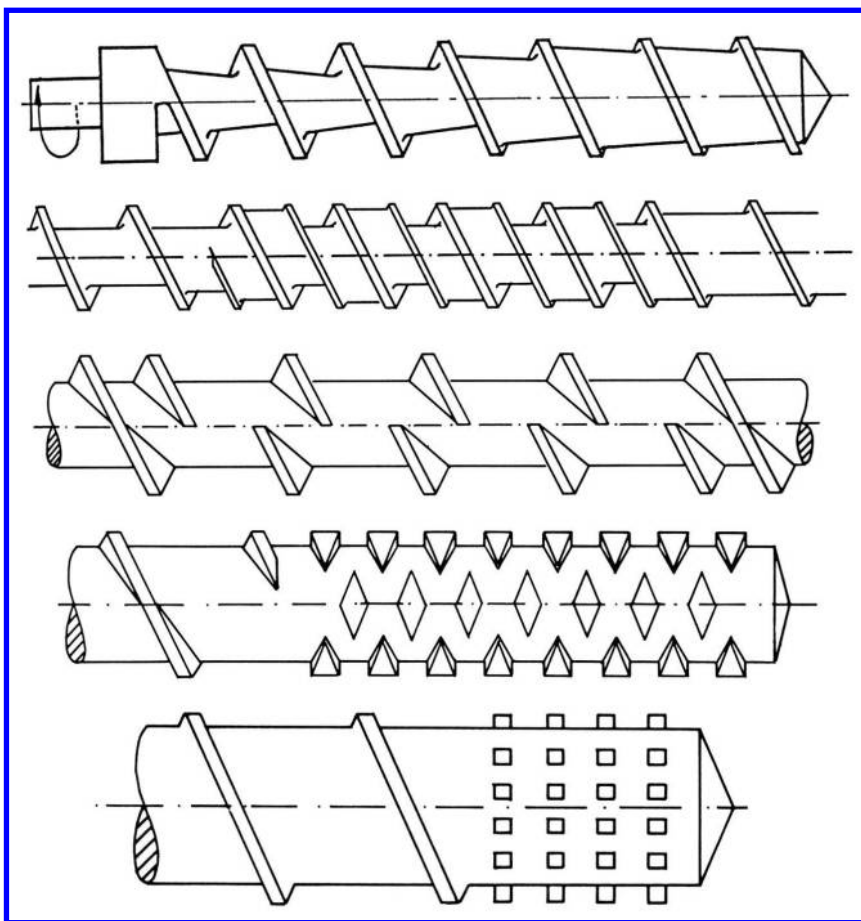


Figure 1-2 Several Types of Thermoplastic Mixing Screws

Some thermoplastic compounds require multi-step mixing. This is required where a high degree of homogeneity is essential and ingredients may require sequential addition to avoid segregation or chemical interactions. For compounds of this type, the intermediate compound is typically extruded into pellets or chopped strips for re-introduction into the mixer and further addition of compounding ingredients.

A Buss mixer is a variation of the screw mixer design in which a long barrel can be configured to allow high shear mixing of ingredients at one end, with separate feed ports for sensitive additives into a less aggressive mixing zone. This design also allows liquid additives to be directly added during compounding. With a traditional screw type mixer, liquids are often added in the form of a mixture with inorganic materials. Figure 1-3 shows a view of a Buss mixer and Figure 1-4 illustrates the internal and external configuration. Polymer compounding with a Buss mixer is a continuous process. Batches are typically defined in context of a campaign wherein a batch of raw materials is used to completion or a particular production target compound weight is met. Precise metering of the raw materials is a key consideration for assuring consistent quality of the thermoplastic compound.

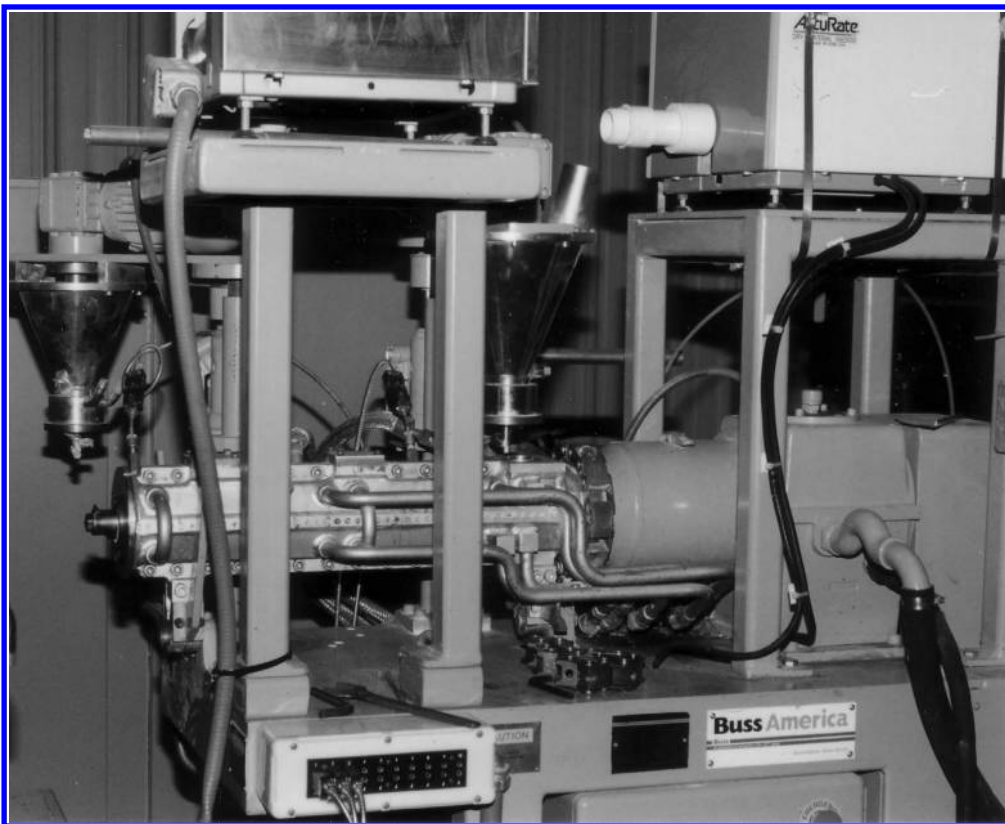


Figure 1-3 Buss Mixer

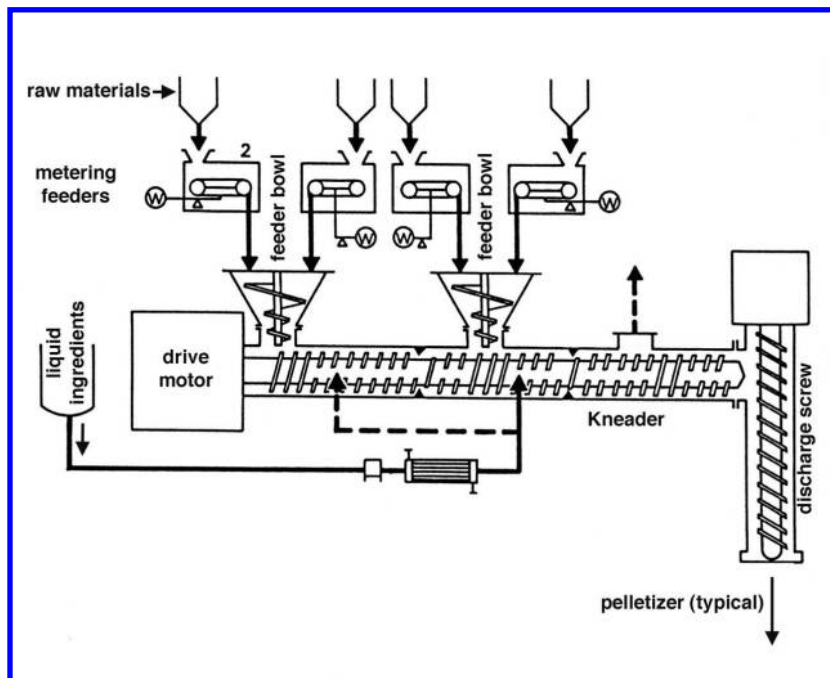


Figure 1-4 Illustration of a Buss Mixer

It is rare to use a Buss mixer for multi-stage compounding operations. In Figure 1-4, the output of the Buss mixer is directly fed into a feed screw machine where high pressure forces the compound through a die or into a pelletizer head.

Multistage Mixing

In some cases, polymers may be compounded from simpler starting compounds formed with two or more of the raw materials. These are identified as master batches and are often prepared when bulk addition to a single stage process would cause them to separate or to alter the bulk polymer properties during mixing to the point where mixing would be inefficient.

Proper dispersive mixing, which focuses on short-range blending of the compound, is achieved through careful selection of the proper mixing screw, mixing temperature, screw rotational speed, back-pressure, sequence of addition, and proper preparation of the raw materials to avoid caking. Distributive mixing, which addresses the overall homogeneity of the batch, is controlled in a single compounding operation by careful and absolutely consistent metering of raw materials. Without a second mixing step, distributive mixing is limited to the volume of compound contained within the mixer barrel. Improved distributive mixing can be achieved where the compound is prepared in two stages.

Mixer Cleaning

Cleaning of the mixer is required between runs and when changing to a different compound. In some cases, the extruder is torn down and the barrel and screws are mechanically cleaned. An alternate method is to run a high-shear cleaning compound through the mixer, followed by a purge period with the new compound before production of the new compound begins. Some types of

compounds with sensitive end-use considerations are isolated to particular machines to protect against carryover risk.

Final Form

Thermoplastic compounds are most commonly supplied in the form of pellets. These are formed by extrusion of the polymer through a strand-forming die plate with a pattern of round holes. This is run under water, in a water-spray environment, or in a chilled airstream. As the hot polymer is extruded, a continuously rotating blade cuts the polymer strands into short segments, thus forming the pellet geometry. With water-cooled pelletizing, the quality of the quench water must be controlled to prevent contamination.

Methods of Compounding: Crosslinked Elastomers

Elastomeric compounds are typically prepared in a two-stage process. The base polymer enjoys a certain level of fluidity, so it typically does not require much heat addition for processing. Since the viscosity is very high and does not lower significantly with temperature, mixing requires very high shear of the ingredients. Mixers contain two intermeshing counter-driven rotors (Figure 1-5) each of which has a complementary lobed or convoluted profile. These profiles serve to shear the compound in the gaps, while also circulating the ingredients. The profiles vary and are recognized typically by the mixer manufacturer, such as Farrell (Figure 1-6), Banbury, Francis Shaw, Werner & Pfleiderer, and others. The rotors are enclosed in a heavy casing since the internal pressure and shear energy are very high. Mixers are water-jacketed so that the frictional heat developed during mixing can be removed through a heat exchanger. With the completely enclosed internal mixer, compounds are prepared in one batch. In other words, all ingredients get introduced and co-mixed in a closed mixing cycle. A variation of this technology will be described later in this chapter.



Figure 1-5 Intermeshing Rotors from Internal Mixer

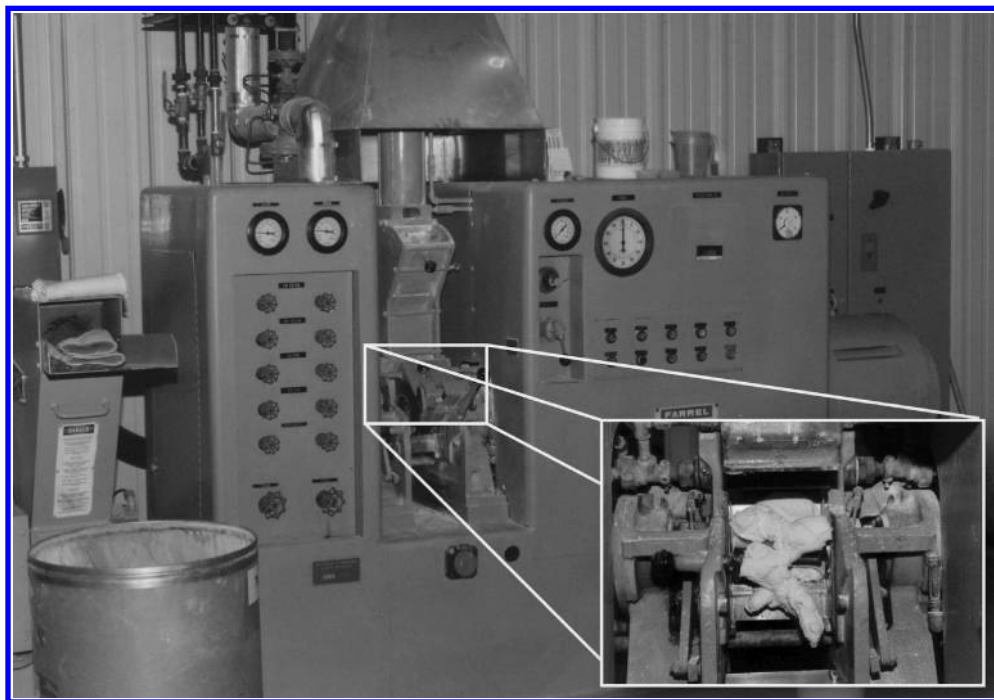


Figure 1-6 Photograph and Close Up of Farrell Internal Mixer

Batch Mixing

Mixing occurs in stages, beginning with the base polymer. This is pressure-fed into the mixer by injection of a bale, strips, or pellets, using a hydraulic or pneumatic ram. The polymer heats and its viscosity reduces, then the inorganic ingredients are added. Processing aids such as carboxylic acids may be added to help reduce shear and to improve wetting of the inorganic compound. If an external antioxidant is needed, this would be added with or before introduction of the reinforcement to protect the polymer against oxidation. Liquid processing aids and coupling agents may be added first to the inorganic so that they are not lost during processing. Due to the extremely fine particle size and low density of carbon black, this is normally added in the form of a high concentration of carbon black in the base polymer or other polymer, separately prepared into a master batch by twin-screw mixing.

In other stages of mixing, additional polymers, waxes, extender oils, and internal lubricants might be added. Addition sequence is driven by melting temperature, viscosity, and thermal stability of the ingredient. Internal mixers are sealed against leaks of high viscosity, cohesive elastomer compounds; however, ingredients in liquid form will not be retained in the mix unless added in master batch form or blended with inorganic ingredients.

In a final mixing step, the crosslinking agent is added. Internal heat generation in the mix must be low enough to prevent the peroxide from decomposing and initiating a crosslinking reaction within the mixer.

Internal mixers must be run in a full or nearly full condition, so a batch recipe is calculated to provide an appropriate volume. If not filled, the ingredients will not be properly sheared and heat transfer will be compromised. Typical commercial mixers have a batch size of at least 100 pounds

of compound. A mixer of this size will have a drive motor of no less than 75 horsepower. Proper dispersive mixing is a balance between proper shear, sequence of addition of ingredients, and thermal stability. Mixers have extensive monitoring instrumentation that provides continuous feedback about thermal conditions, rotor torque, and rotor speed. Once a mixing process has been developed, a standard protocol is followed for preparation of the compound.

An internal mixer provides the shear necessary to mix a raw elastomer with its compounding ingredients. It is imperative that the compound is homogeneous throughout the batch so that its properties are uniform. For distributive mixing, a second stage of mixing is used. In many cases, an internal mixer is mounted above a two-roll mill (Figure 1-7) and when mixing is completed a bottom hatch is opened, allowing the compound to fall onto the two-roll mill. In other cases, the compound will be transported to the mill.

Processing

A two-roll mill consists of two large-diameter counter-rotating cylinders, with a variable gap between them. The rolls are maintained at a fixed temperature through internal fluid heating and an external heat exchanger. The elastomer compound forms a sheet on the roll surface. This is continuously cut into wide strips by the operator, folded over, and placed back on the rolls. This process is repeated for perhaps 15 minutes to assure that the compound is fully homogenized.

In some cases, the curing agent is added during the milling operation, generally in the form of a master batch. This practice is used for peroxides that decompose at a lower temperature, to reduce the risk of accidental curing in the internal mixer, when localized temperature can be very high.

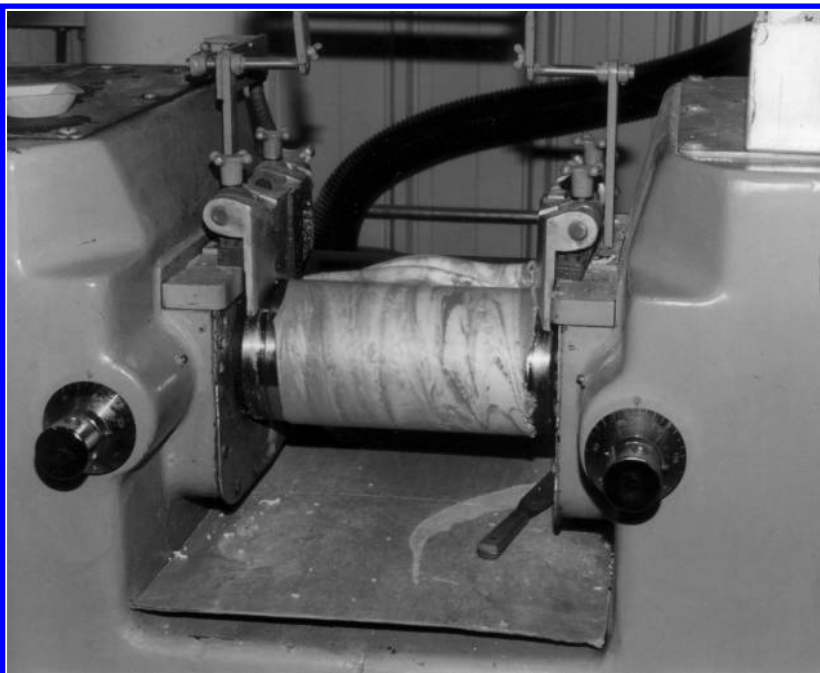


Figure 1-7 Laboratory Scale Two-Roll Mill

With a closed mixer, control of distributive mixing is inherently good, since all materials are added in a single batch and mixing occurs in two stages. Failure to add an ingredient or to improperly treat raw materials may lead to dispersion and homogeneity problems.

Continuous Mixing

A second type of elastomer compounding makes use of a continuous mixer. This type of machine is most often used where a high volume of rubber compound is required to feed large production lines for applications that include tires, sheet rubber products, cable insulation, hoses, belts, and others. Figure 1-8 is an illustration that shows the internal configuration of a continuous mixer. This is a hybrid design that features a feed screw, similar to a screw type mixer that feeds raw materials into a heated high shear rotor type mixer. As shown in this figure, raw materials are fed continuously and mixed compound is continuously discharged. Control of dispersive mixing is achieved by designing a process that optimizes residence time in the mixer, rotor speed, temperature, and rotor profile. Continuously blended rubber compound is typically transferred directly to a two-roll or calendaring mill for distributive mixing.

Since internal mixers can be opened for material feed and compound removal, these are generally simpler to clean when compared to screw-type mixers. It is a common practice to run natural rubber or special high-tack, cohesive compounds through a mixer as a final stage of cleaning. Further, the first batch of compound is typically sacrificed or saved for experimental work following clean-out.

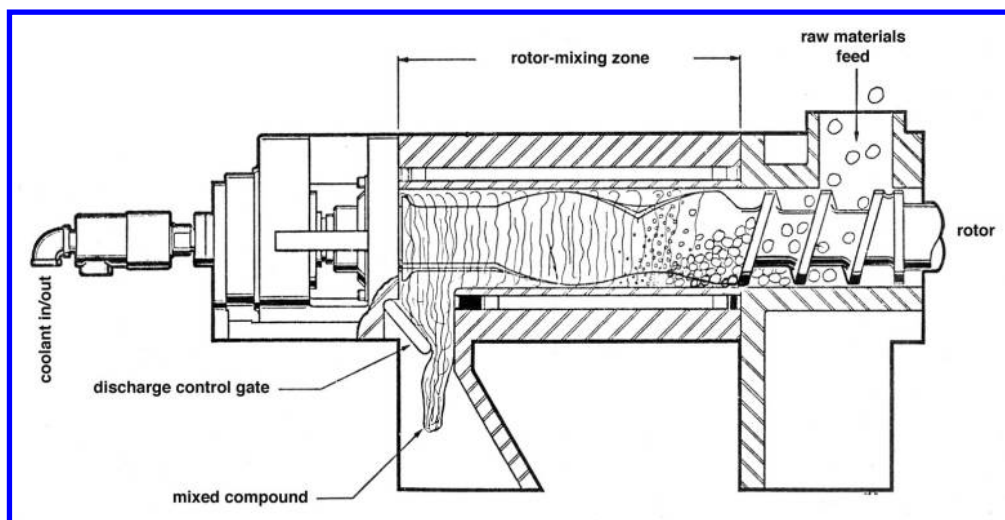


Figure 1-8 Continuous Mixer for Elastomer Compounding

Mixer Cleaning

Cleaning of the two-roll mill is a simple operation since the compound only contacts the exposed external surface of the rolls. Typically a natural rubber compound may be used for surface cleaning and/or the first batch of polymer compound might be used for this purpose.

Intermediate Forms of Compounds

Strips of elastomer compound can be manually or automatically cut directly from the milling operation and placed into release packaging. In other cases, the warm compound might be placed directly into an extruder where it is pressed through a cylindrical or rectangular die and cut into short sections or coiled for subsequent use. In all cases, non-crosslinked rubber compounds cohere strongly; therefore, a release agent (anti-blocking compound) or physical method is required to maintain a manageable form of the compound. Surface treatment options are significant. These may include water baths with talc, direct application of talc, treatment with the same inorganic in the compound, surface wetting with silicones, and others. Physical treatments include release films, physical separation of pre-forms onto release layers, or packaging into trays that prevent contact between pre-forms.

The more amorphous grades of elastomer compounds tend to have high surface tack before crosslinking, so the elastomer in the form of pellets tends to form an inseparable bond between pellets. Blocking can be reduced by the addition of an inorganic anti-blocking ingredient, such as talc. This is generally added in a water slurry, so that the talc coats the exterior surface of the compound with a very thin layer. Surfactants are often used to enhance talc coating of the surface. In some cases, organic anti-blocking agents are used.

Prior to crosslinking, softer grades of elastomer compounds flow slowly, so these cannot be produced in a form that is unconstrained. A common intermediate form of such compounds is long, continuous ribbons that are dusted with a release agent and coiled. Sheets or other forms can also be hot-pressed, dusted, and shipped with release packaging that helps to separate the layers for subsequent processing. In still other cases, the elastomer compound is wrapped into a polyethylene sheet to hold its shape and to protect against contamination. In this approach, the elastomer bonds to the packaging material and both are blended in the final extrusion operation.

Final Form

Crystalline forms of elastomer compounds can be produced into pellet form in some cases. These are typically pressed in a compression molding operation or in a continuous molding press, resulting in pellets that are about 0.5 inch diameter. If a compound has a high density, it may retain its shape sufficiently to allow it to be packaged into gaylords in pellet form. Contracted forms are often supplied from compounders to molders. The latter might specify compounds in the form of molded disks, which can then be fed directly into molding machines where the final forms are produced and crosslinked.

Extraction and Analysis

Introduction

A significant focus throughout this Handbook is that the identification, classification, and suitability of additives directly affect the cost and performance of end-use products. Included in these considerations are product quality, lot-to-lot reproducibility, production control, and product aging/weathering. A particular additive may be comprised of several components; however, only the major ingredient is identified in the description or MSD disclosures. Therefore, it is important also to know the composition and purity of the additives themselves. This is best achieved by developing and/or acquiring an inventory of well-defined standards.

As discussed in an earlier section of this Handbook, additives may contribute to extractable and leachable compounds. Other sources include base polymer breakdown products and/or primary formulation ingredients and their breakdown products. These and other extraneous compounds comprise the basis for the extraction, analysis, and identification methods described in this chapter.

The authors have seen numerous examples of additive-associated problems that have been traced to poorly characterized materials employed at the front end of the design and production cycle. The use of such materials can result in serious legal and/or liability problems for the product manufacturer. Additionally, the use of plastics additives is becoming a target for scrutiny by regulatory (i.e., FDA, CPSC) and environmental (EPA) agencies (e.g., food-related materials). In response to this heightened scrutiny, there is increased interest in the identification of potentially problematic additives and materials prior to the manufacturing of the end product. Ensuring the proper material pedigree through the design and implementation of a comprehensive sampling and testing plan reduces the possibility of using unsuitable raw materials. The analysis methods and principles described in this chapter will provide the analyst with the tools to accomplish this task. Case studies highlighting applied examples are presented in Chapter 10.

Extraction Methods

The above factors have proven to be justification for the development and implementation of a variety of extraction methods which have been reviewed periodically (1-6).

[Table 2-1](#) lists methods commonly used to extract extraneous compounds from various types of plastics/polymers.

As seen in [Table 2-1](#), extraction methods are divided into two basic groups: liquid/solid extraction and thermal desorption. Both groupings may employ sample preparation techniques such as grinding or cutting to increase surface area and improve extraction efficiency. Thermal desorption has the combined advantages of minimal sample preparation plus elimination of solvent selection and extraction prior to analysis.

Table 2-1 Extraction Methods for Additives

Method	Comments	References
Preparation: Grinding and Cutting of Plastics	Increase the surface area via ball mills/cutting mills — ambient or cryogenic temperature. Suitable for liquid/solid and thermal desorption methods.	(2)
Dissolution/Reprecipitation	Dissolution of plastic in suitable solvent or solvent system. Direct analysis or precipitation of polymer with non-solvent.	(2), (5)
Sonication*	Use of ultrasound energy to agitate the plastic, releasing additives. * Solutions must be filtered to remove possible particulates.	(8)
Soxhlet Extraction — Traditional and Improved (i.e., Randle)	Solvent extraction of solids — choice of solvent or solvent system.	(5), (9)
Focused Microwave Assisted Soxhlet Extraction (FMASE)	Water is used as the extractant in the application of focused microwaves to enhance the extraction.	(10)
Accelerated Soxhlet Extraction	Sample is extracted with a suitable solvent at elevated temperature and pressure.	(11)
Supercritical Fluid Extraction	Use of supercritical fluid CO ₂ to solubilize and extract additives.	(12)
Pyrolysis GC/MS	Pyrolysis of polymers and additives identified by interpretation of MS pyrograms.	(13)
Thermal Desorption (indirect)	Thermally desorb additives into traps or directly onto chromatography column.	(14)
Thermal Desorption (direct)	Vacuum/thermal desorption/extraction via direct MS direct insertion probe — no separation.	(5)
Thermal Desorption (direct)	Direct thermal desorption from sample located within the injection port liner (see discussion below).	(15)
Thermal Desorption (direct)	Direct thermal desorption from sample located within a sample tube of modified GC inlet.	(16)

Efficient extraction of the extraneous compounds is important for accurate compound identification and essential in attempts for quantification. Realistically, however, factors attributed to both the plastic/polymer matrix (non-homogeneous mixing of the additives) as well as the extraction

methods employed (insolubility, decomposition, rearrangement, and/or loss during the extraction) make accurate quantitative analysis a difficult goal to achieve on a routine basis.

While the inherent thermal decomposition of some additives such as UV, visible-light stabilizers has initiated the development of less destructive techniques like supercritical fluid extraction (SFE), it does not preclude the use of thermal desorption methods. In practice, the thermal decomposition products from the additives can be used to assign an identity to a particular compound.

The authors have developed a thermal desorption technique based on the heat of a gas chromatograph (GC) injection port. In this technique, a plastic/polymeric sample is placed into the injection port liner (Figure 2-1). In our Agilent GC/MS system, we utilize a split liner with an inside cup (Agilent part number 18740-80190). For ease of handling, and to improve the efficiency of the technique, we have installed the agilent flip top inlet sealing system to the 6890 GC of our Agilent GC/MS system. For lower molecular weight plastic samples, we insert a loose-fitting plug of aluminum foil into the liner ahead of the sample to prevent melted plastic from flowing into the cup portion of the liner. In addition to prolonging the use of a liner, it prevents any melted material from fouling the injection port and/or the GC column during the analytical run. Although we prefer this liner, there are a number of configurations offered by suppliers that would satisfy the requirements of this technique. There also is a commercially available GC inlet (Gerstel GmbH & Co. K.G.) for direct thermal desorption of solid samples (Ref. 16 in [Table 2-1](#)).

Monitoring the injection port temperature or the desorption temperature of the commercial inlet is imperative. An overly high temperature can result in thermal degradation of the sample and create invalid pyrolysis products. A case study illustrating this potential problem is presented in Chapter 10.

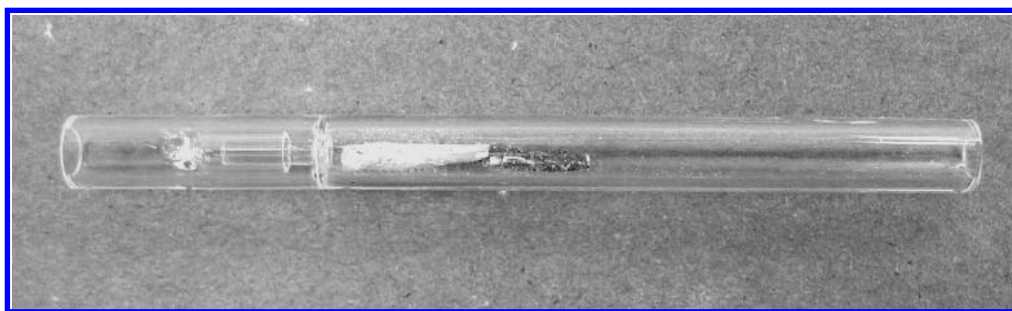


Figure 2-1 Plastic in Injection Port Liner

The heat from the injection port liner combined with the GC column flow causes the volatiles contained in the sample to be thermally desorbed directly onto the GC column. This reduces or eliminates interfering components of the sample matrix. An example of this “additive specific” extraction is shown in [Figure 2-2](#). This technique also can be used to obtain the purity and identity of neat additive standards that are not readily soluble. By altering the injection port temperature, an analyst can extract various types of additives without thermally degrading the sample matrix. There

are no limitations on the additive/polymer combinations that can be analyzed. Another advantage of this technique is that it requires only a few milligrams of sample; typically 2 to 5 milligrams per analysis..

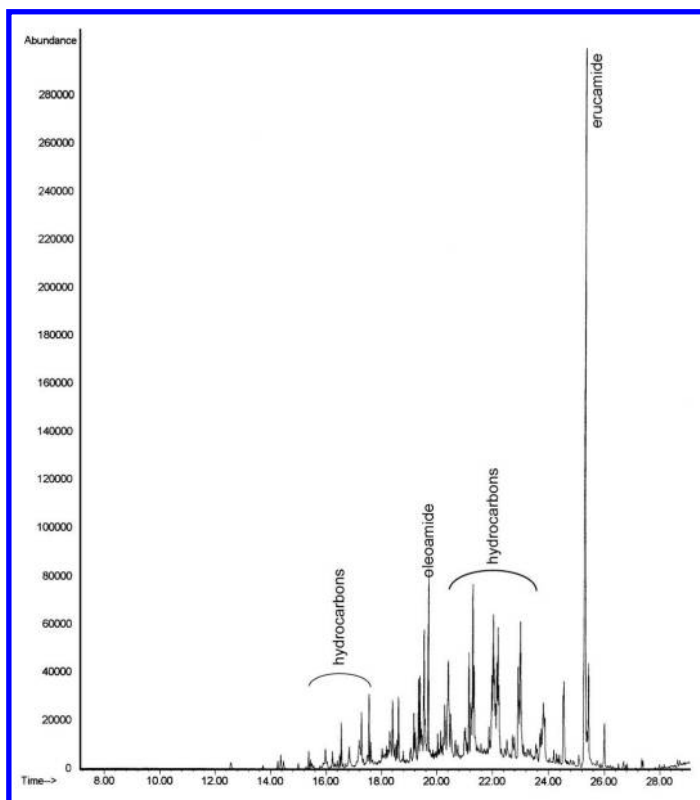


Figure 2-2 Additive Specific Extraction of a Polyethylene Plastic Bag

In addition to being an efficient and reliable extraction technique for the qualitative analysis of additives from a variety of plastic/polymeric matrices, there are additional applications where this technique can be used to provide information on the sample matrix. Sequentially increasing the extraction temperature (injection port temperature) can provide insight into the efficiency of the polymer cross-linking process without resorting to the destruction (pyrolysis) of the sample. Also, the thermal stability of the polymer/additive interaction can be monitored. This can result in an approximation of thermal aging and thermal decomposition of the plastic/polymer matrix. The authors have used this approach when studying underground cable failures.

Analytical Methods

The emphasis of this work is on the analysis of plastic additives through gas chromatography/mass spectrometry (GC/MS). GC/MS systems are a common analytical tool in quality control and analytical service laboratories; and electron impact (EI) mass spectra are recognized as reliable data for the identification of organic compounds. Traditional methods have employed a flame ionization detector (FID) with identifications based solely on GC retention time data. These methods lack the specificity necessary to distinguish between components attributable to the sample matrix or the additive.

Of course, there are additives which may require an inorganic analysis technique. An example is shown in Figure 2-3, which depicts the energy dispersive spectroscopy (EDS) spectrum of Akro fax A, elemental sulfur. However, most additives are based on organic compounds and are suitable for GC/MS analysis. The main weakness of this technique is the maximum molecular weight limit since a number of additives possess molecular weights in excess of 1000 daltons. This shortcoming has been addressed by recent advances in both quadrupole and time of flight GC/MS instruments, which have extended upper ranges above 1000 daltons.

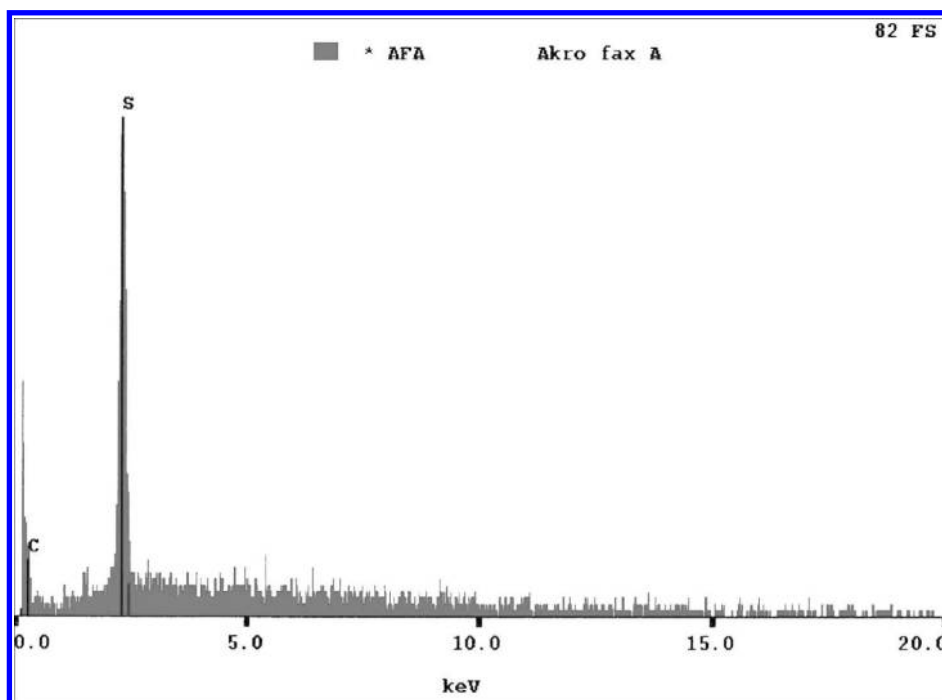


Figure 2-3 Energy Dispersive Spectrum — Elemental Sulfur

Despite the fact that a molecular ion cannot be attained for some additives, the characteristic ion fragmentation pattern can be used to classify the type of additive used. An example of this is illustrated in Figure 2-4, which depicts a (di-tert-butyl-4-hydroxyphenyl) propionate moiety of Ethanox 310. Several antioxidant additives are based on this type of structure. Without identifying the molecular ion of the molecule, an analyst can establish the fact that a substituted propionate type of antioxidant is present in the material. This premise is the basis for the value of the MS data.

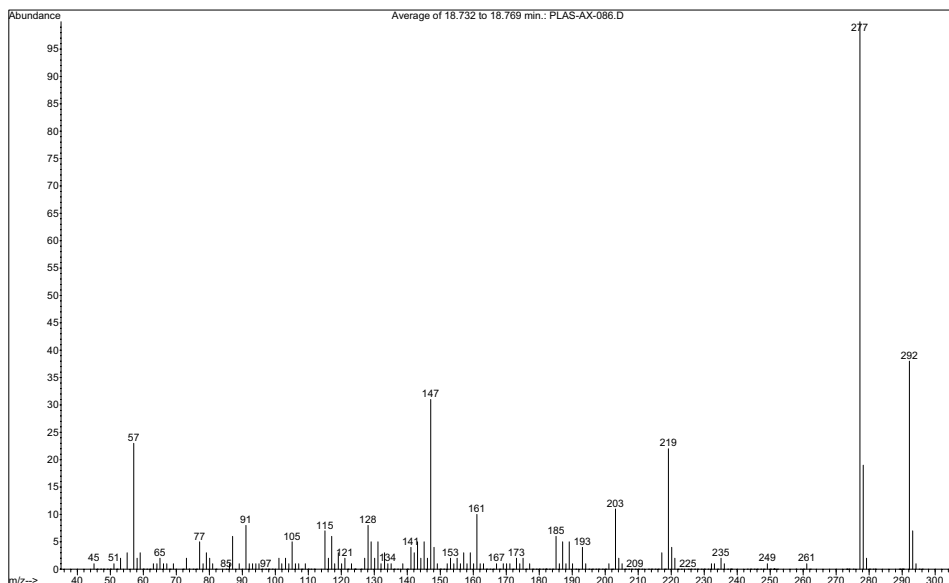


Figure 2-4 Ethanox 310 Propionate Moiety

Instrumental Conditions

All standards and “real-world” samples were chromatographed using a 30 meter, 0.25 mm i.d., 0.25 micron film MS-5 column (QuadRex Corporation, Bethany, CT).

The additive standards for the MS library were dissolved in a suitable solvent and a sample was injected into the GC/MS system, or a sample was transferred into an injection port liner as is done for “real world” samples. Additive standards were run at temperature program rates of 10 °C or 15 °C due to the lack of the necessity for multi-component separation. The actual temperature program used is listed on each Total Ion Chromatogram (TIC).

GC conditions for all standards:

- Injection port: 220 °C
- Temperature programs: 50-330 or 340 °C
- Temperature. program rates: 10 or 15 °C

MS parameters:

- MS transfer line: 310 °C
- MS source temperature: 230 °C
- Threshold: 500
- MS mass range: 45-1000 daltons

Determining the instrumental conditions for “real world” samples involves some trial-and-error. As was discussed earlier in this chapter, the injection port temperature is critical for the success of this extraction technique. The authors have achieved good success for most samples with injection port temperatures in the 180-220 °C range. In our experience a starting oven temperature of 50 °C is adequate to reveal any lower boiling range compounds; and a temperature program of 8-10 °C/minute provides sufficient chromatographic resolution for all but the most degraded samples. We

have found that with most analytical runs, it is advantageous to perform baseline subtraction. This ensures cleaner mass spectra and more accurate compound identifications.

Sample Size of “Real-World” Samples

A sample size of 2 to 5 mg produces enough data to obtain a good chromatographic and MS profile of any additives. In cases where a large amount of the plastic/polymer is analyzed, multiple samples should be done to ensure the homogeneity of the sample matrix.

System Maintenance

Gas Chromatograph

Although good laboratory practices dictate a comprehensive scheduled maintenance program, plastic/polymer and additives samples present a unique problem. They include a broad range of materials and chemicals that have a variety of physical properties, and obtaining accurate analytical results requires diligent instrument maintenance and an adequate consumables budget. Compounds that are easily soluble in an organic solvent can foul both injection port liners and GC syringes when injections are made. Cleaning syringes immediately after use ensures that the syringe barrel and/or needle will not become plugged. Some plastic/polymer samples could melt into the retainer cup of the liner, which renders it unfit for further use. Consequently, we like to keep 8 to 10 clean and silanized liners ready for sampling. Liners should be cleaned on a regular basis. After each analysis, we use organic solvents in an ultrasonic bath to remove any sample/additives residue. This is followed by heating to 300 °C for 30 minutes. All liners are silanized after several cleanings to ensure that there is minimal interaction between the sample and the glass surface. Depending upon the type of GC used, it also may be necessary to change the injector seal and washer as they come into contact with the volatiles from the sample. Split vent lines should be cleaned periodically to prevent carry-over and the presence of “ghost” peaks from one sample to another. We routinely cut 2 to 3 inches from the injector end of the GC capillary column. Since resolution is a function of the square root of the theoretical plates, loss of column resolution is minimal. However, retention data windows, if utilized, must be changed at regular intervals. When large amounts of compounds are deposited on the column, we routinely perform a blank run before the next analytical run. Finally, we also rinse the GC column periodically to remove insoluble components. We use an alternate column during this process to decrease instrument downtime.

Mass Spectrometer

The physical properties of plastic/polymer matrices and additives samples combined with the high GC column temperatures result in the mass spectrometer ion source becoming dirty more quickly than with typical usage.

To limit instrument downtime, and if financially feasible, it is a good idea to have an extra ion source which can be exchanged after venting the instrument. This encourages more frequent source maintenance and provides more consistent analytical results.

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Crosslinking Compounds/Accelerators

The chemical crosslinking process has its origins in the Goodyear process by which rubber was transformed from a viscous form into a shape-retaining rubbery material through reaction with sulfur and heat. This 'vulcanizing' process promoted bonding between unsaturated end groups in the natural rubber chains, thus forming 'crosslinks' between chains. With these crosslinks, the rubber molecules were no longer subject to mutual slip, thus a molded object would permanently retain its shape while retaining elastomeric behavior.

Crosslinking is a major commercial process for elastomeric, thermoplastic, and liquid polymeric materials. The approaches for crosslinking reaction initiation vary with the type of polymer, the end application, costs, and technical approach. Many crosslinking processes are thermally initiated. Heat exposure increases oxidation risk, while considerably boosting energy requirements. The rate of crosslinking can be increased by careful technical development of a process and selection of organic compounds that function as cure accelerators. In some cases, the rate of cure may be moderated with chemical retarding agents to control exothermic reactions and physical stability.

Crosslinking of many commercial thermoplastics is conducted with reactive peroxides, including dicumyl peroxide, benzoyl peroxide, and many others, all of which have different activation temperatures. At the crosslinking initiation temperature, the peroxide decomposes and forms free radicals that react with unsaturated end groups on the polymer chains, thus forming chemical crosslinks between chains. For thermoplastic addition, stability of the peroxides is increased for storage and handling by incorporation into master batches that may include waxes, clay, fatty acids, or resins.

A wide range of liquid polymers are crosslinked with reactive peroxides, such as benzoyl peroxide, diacyl peroxide, and various peroxyesters and peroxyketals. These are used to crosslink acrylic resins for a wide range of applications. Since these peroxides are inherently unstable, they are reduced in concentration for safe storage and use by dilution with cyclohexane, diallyl phthalate, or dimethyl phthalate. These diluents must be understood from an analytical perspective for proper role and source identification.

Crosslinking of many thermoplastic polymers can be accomplished by addition of a vinyl silane. In this process, the vinyl silane is mixed into the polymer during extrusion. The heat energy grafts the silane to the polymer chains. The component is then molded or extruded into the desired form. Following this, the crosslinking process is initiated by exposure to moisture and heat. With this process, the processing temperature is reduced. Therefore, the polymer is not oxidized and the vinyl silane is not decomposed into a host of reaction products. Analytically, silane crosslinking initiators can be identified by the vinyl silane signature.

Ionizing radiation is used to crosslink a number of rubber and thermoplastic materials, particularly for applications where precise control of crosslinking density (the proportion of crosslinked to non-crosslinked chains in a given polymer) must be carefully controlled and where chemical purity is a key consideration. Polymers for biomedical applications are typically radiation crosslinked. With this process, an electron beam or gamma radiation source is used to provide ionizing energy. Crosslinking proceeds spontaneously if the polymer contains reactive end groups or if an unsaturated copolymer or unsaturated polymer additive is blended. For rubber compounds, diene

monomers are typically added to provide unsaturated bonds. From an analytical perspective, radiation-crosslinked polymers may contain few chemical signatures that indicate the curing process.

Ultraviolet (UV) crosslinking of polymers is broadly used for many applications where heating is impractical or damaging to the base polymer and where other forms of ionizing radiation may be harmful or excessively costly for the application. UV radiation can be used to decompose a reactant that is blended into a polymer and the free radicals that result will form crosslinks in the polymer. UV curing is used for a wide range of urethanes for cured-in-place coatings, for example. This method is also commonly used for acrylic composite dental restoratives. The crosslinking initiators used for this process must strongly absorb UV radiation and they must be stable and have low volatility in the polymer prior to crosslinking initiation. Benzophenones are a major class of organic compounds used for this process.

Rigid polymers such as epoxy and polyurethane are used in high volume for a wide range of structural, coating, electrical, and other applications. Epoxy formulations vary widely and the chemical signatures of cured resins will vary accordingly. Amine curing agents are the most commonly used for epoxy systems. The selection of the type of amine affects the rate of cure and also impacts the end use of the crosslinked material. Amine-crosslinked epoxies have increased moisture sensitivity compared to those cured with aromatic isocyanates, for example. The amine crosslinking agents include triethylenetetramine, ethylenediamine, diethyltriamine, cycloaliphatic amines, and others. Analytically, these amines might be identified through GC/MS analysis of solvent-extracted or thermally desorbed samples, particularly if unreacted amines remain.

Polyurethanes are also available with a wide range of crosslinking systems, some of which are extremely sensitive to UV exposure. One such curing agent is toluene diisocyanate. Hexamethylene diisocyanate is not subject to UV-induced degradation. As with epoxies, urethanes are highly crosslinked and analytical determination of the ingredients and extractible organics requires careful selection of methodology and knowledge of the polymer systems.

From an analytical perspective, the crosslinking materials and process should be well understood. A reactive peroxide, for example, will generally not be evident in the analysis of a polymer crosslinked with this material. This will be evident when not fully decomposed during a cure process, for example, and the presence of non-reacted peroxide may be a valuable indication of an under-cure condition. Typically, the decomposition products of dicumyl peroxide are what will be found analytically. These include acetic acid, cumyl alcohol, acetophenone, and others. Heating of most thermoplastics to a level that initiates decomposition of the curing agent would also oxidize the base polymer. It is therefore necessary to protect the polymer with an antioxidant. GC/MS analysis of a typical peroxide-crosslinked polyethylene will reveal the peroxide decomposition products, an antioxidant, and no trace of the original peroxide.

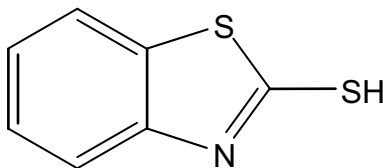
Accelerators

The rate of crosslinking of commercial rubber products and a number of other thermosetting plastic compounds can be accelerated by addition of a number of compounds identified as cure accelerators. These are useful for increasing throughput in commercial processes, for locking in transient foam structures, and for controlling recovery in shape-retaining components. These are also useful when a crosslinking agent must be used at the lowest possible temperature to prevent decomposition of the polymer. Accelerators may also enhance tensile properties and improve age resistance of the final product. Cure accelerators are also known as crosslinking synergists.

Most accelerators are organic substances that contain either nitrogen or sulfur, or both. Typical accelerators include tetraisobutylthiuram disulfide, n-oxydiethylene thiocarbamyl-N-oxydiethylene sulfonamide, tetrabenzylthiuram disulfide, and others. They can be classed as either primary or secondary accelerators and are often used in combination, depending on the desired final outcome. Crosslinking of many commercial thermoplastics is conducted with reactive peroxides, including dicumyl peroxide, benzoyl peroxide, and many others, all of which have different activation temperatures. At the crosslinking initiation temperature, the peroxide decomposes and forms free radicals that react with the unsaturated end groups on the polymer chains, thus forming chemical crosslinks between chains. For thermoplastic addition, stability of the peroxides is increased for storage and handling by incorporation into master batches that may include waxes, clay, fatty acids, or resins.

Accelerator MBT, MBT/MG

Akrochem Corporation

**CAS Number** 149-30-4**RTECS Number** DL6475000**Abbreviation** 2-MBT**Formula** C₇H₅S₂N**Molecular Weight** 167.25**Chemical Name**

2-mercaptobenzothiazole

Synonyms

2-benzothiazolethiol; 2-benzothiazolylmercaptan; 2(3H)-benzothiazolethione

Brand Names & Manufacturers

Captax/Rotax (purified form)

R.T. Vanderbilt Company

Perkacit® MBT

Akzo Nobel Chemicals B.V.

Thiotax

Solutia, Inc.

Physical Properties**Appearance** Off-white to yellow powder**Melting Point** 180-182 °C**Boiling Point** 260 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH 2.0	Acetone 10.0	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application** Used as a vulcanization accelerator for rubber mixes based on natural and synthetic rubbers and in the production of plastics and lacquers.**Regulatory Information**

FDA approved 1998 for the following materials to be used in contact with food: adhesive preservatives, 21CFR175.105; a rubber accelerator (up to 1.5% of weight of rubber), 21CFR177.2600; in the synthesis of slimicides for use in paper/paper-board, 21CFR176.300; an adjuvant in the manufacture of foamed plastics, 21CFR178.3010. Listed in 40CFR136.1 and USEPA Method 640: The Determination of Mercaptobenzothiazole in Municipal and Industrial Wastewaters.

Environmental Impact

Does not biodegrade in river water in 8 weeks. Slightly susceptible to indirect photolysis. Medium to low mobility in soil, and marginal to no mobility in sediment. This substance may be hazardous to the environment; special attention should be given to fish. Log Pow value of 2.41 indicates a low potential to bioaccumulate.

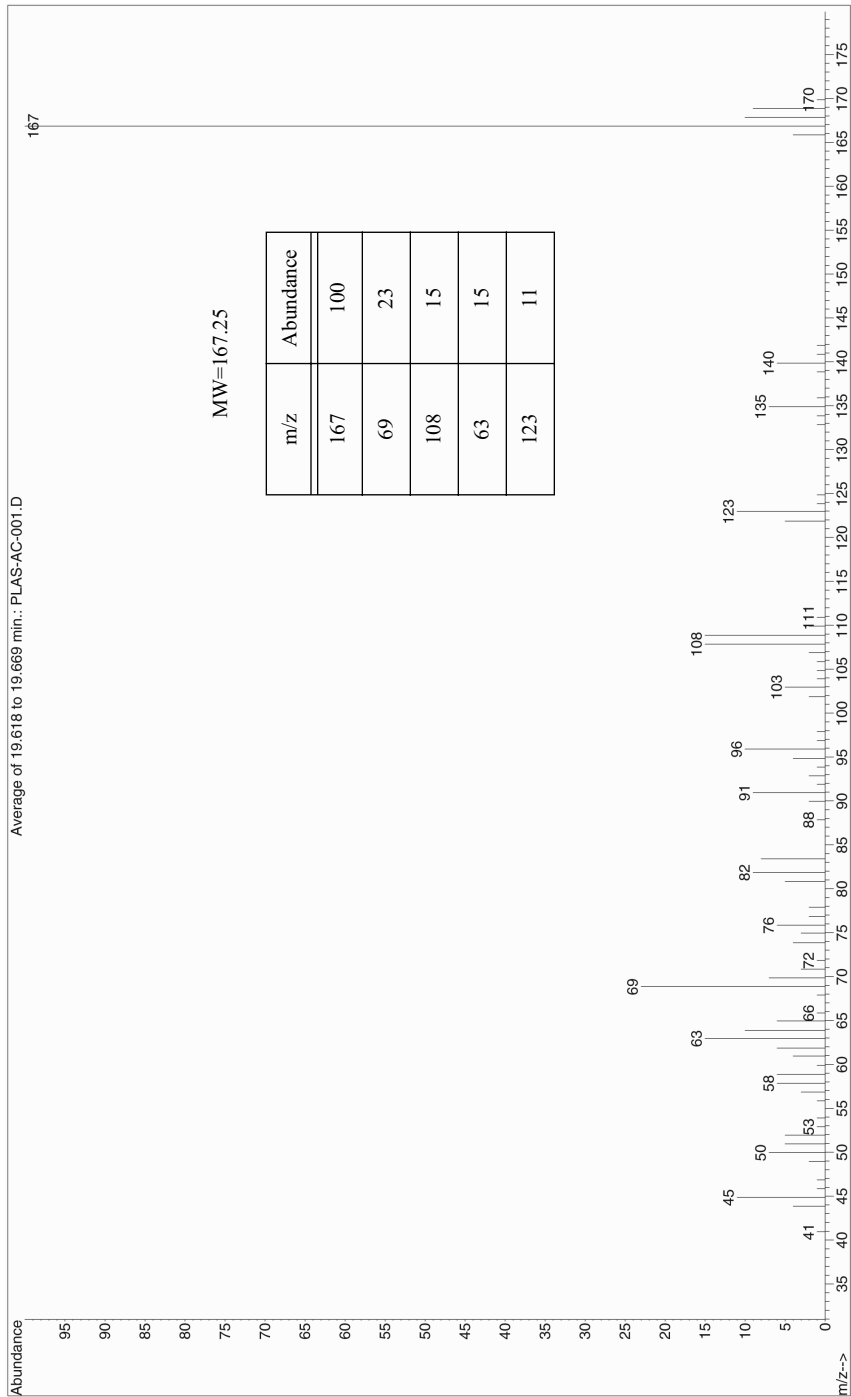
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

A 2-year NTP study on rats indicates evidence of carcinogenic activity in rats gavaged with 750 mg/kg BW (male) and 375 mg/kg BW (female). No carcinogenic effect on bacteria and yeast cells.

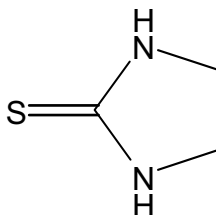
Mass Spectrum for Accelerator MBT, MBT/MG - PLAS-AC-001



For Chromatogram See Appendix A - PLAS-AC-001 - page 445

Accelerator ETU-22 PM

Akrochem Corporation

**CAS Number** 96-45-7**RTECS Number** NI9625000**Abbreviation** ETU**Formula** C₃H₆N₂S**Molecular Weight** 102.11**Chemical Name**

ethylene thiourea

Synonyms

2-imidazolidinethione; 2-imidazoline-2-thiol; 2-mercaptoimidazoline

Brand Names & Manufacturers

Pennac [®] CRA	Pennwalt Corp.
Nocceler [®] 22	Ohuchi Shinko Co., Ltd.
Soxinol [®] 22	Sumitomo Chemical Co., Ltd.
Vulkacit [®] NPV/C	Lanxess Deutschland GmbH Ltd.

Physical Properties

Appearance	White powder					
Melting Point	203 °C			Boiling Point	347.18 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water ~2	MeOH 10-40	EtOH 10-40	Acetone <0.1	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application ETU is used as an accelerator in the vulcanization of polychloroprene (Neoprene) and other elastomers; for coated fabrics, for epichlorohydrin, and for chlorosulfonated polyethylene rubbers. It is also an intermediate for antioxidants, insecticides, fungicides, dyes, pharmaceuticals, and synthetic resins.

Regulatory Information

FDA: Use of ETU as a food additive is prohibited. EPA (1995): Health Advisory for long-term exposure is 0.4 mg/L. Can be monitored in water by EPA Method 509 - Determination of Ethylene Thiourea (ETU) in Water Using Gas Chromatography with a Nitrogen-Phosphorus Detector. FAO/WHO (1993): ADI: 0.004 mg/kg BW.

Environmental Impact

ETU is a trace contaminant and metabolic degradation product of a widely used class of ethylene bisdithiocarbamate fungicides such as Maneb and Zineb. Half-life in H₂O is 7–13 days. Octanol/water partition coefficient as log Pow: -0.66 (calculated).

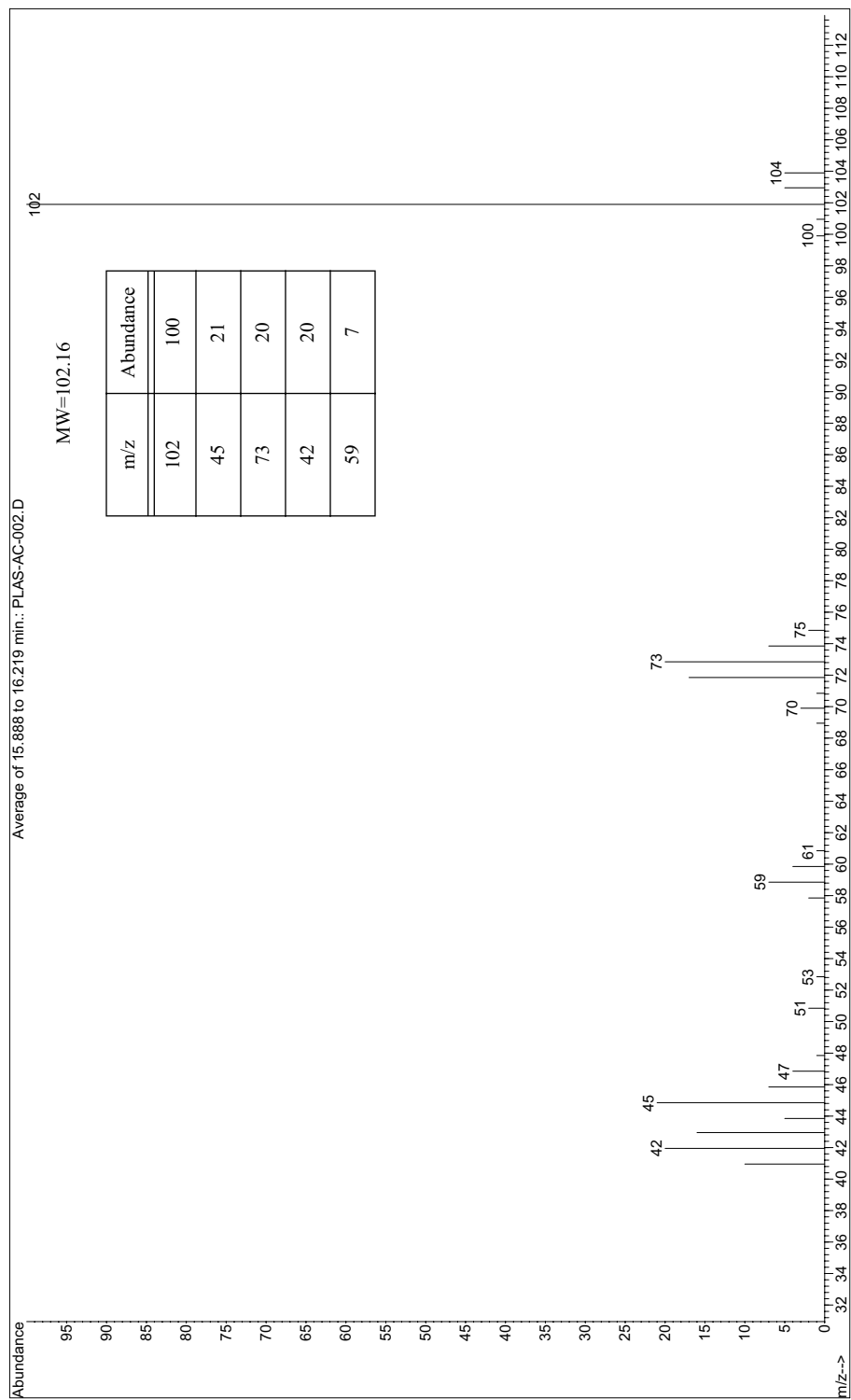
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Ethylene thiourea is toxic and known to produce thyroid neoplasms (thyroid hyperplasia) in rats and liver neoplasms in mice following long-term administration; NIOSH: potential occupational carcinogen; NTP: Suspect carcinogen; OSHA: Possible suspect carcinogen. Acute oral toxicity (LD50): 1832 mg/kg [Rat].

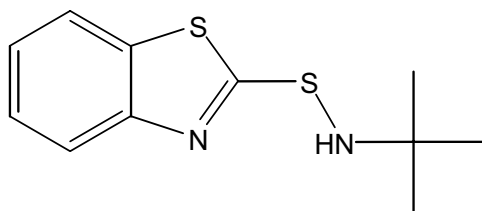
Mass Spectrum for Accelerator ETU-22 PM - PLAS-AC-002



For Chromatogram See Appendix A - PLAS-AC-002 - page 442

Accelerator BBTS

Akrochem Corporation

**CAS Number** 95-31-8**RTECS Number** DL6200000**Abbreviation** TBBS/BBS**Formula** C₁₁H₁₄N₂S₂**Molecular Weight** 238.38**Chemical Name**

N-(1,1-dimethylethyl)-2-benzothiazolesulfenamide

Synonyms

N-(1,1-dimethylethyl)benzothiazolesulfenamide; benzothiazolyl-2-tert-butylsulfenamide; benzothiazyl-2-tert-butylsulfenamide

Brand Names & Manufacturers

Delac [®] NS	Uniroyal Chemical Co.
Pennac [®] TBBS	Pennwalt Corp.
Perkacit [®] TBBS	Akzo Nobel Chemicals B
Santocure [®] NS	Solutia Inc.

Physical Properties

Appearance	Cream to buff powder or pellets					
Melting Point	105 °C	Boiling Point		Not available		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water 0.345	MeOH U	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane U

Application**Application, Regulatory & Environmental Information**

TBBS is used as a vulcanization accelerator in NR, SBR, BR, and rubber blends. Normally used alone or with small quantities of ultra accelerators in tire compounds or other industrial rubber products.

Regulatory Information

FDA approved 1998 for use as an accelerator in the manufacture of rubber material intended for use in all stages of production, processing, packaging, and transport of food: 21CFR177.2600.

Environmental Impact

TBBS does not ionize at environmental pHs, is not readily biodegradable, but hydrolyzes in less than 1 day at pH 9 or less. The identified hydrolysis products: mercaptobenzothiazole, di(benzothiazoyl)disulfide, t-butylamine, and benzothiazole are non-volatile, with a low potential for bioaccumulation, and are not readily biodegradable. Indirect photo-oxidation by hydroxy radicals is predicted with a half-life estimated at 2.8 hours. Log Pow of 3.9 at room temperature.

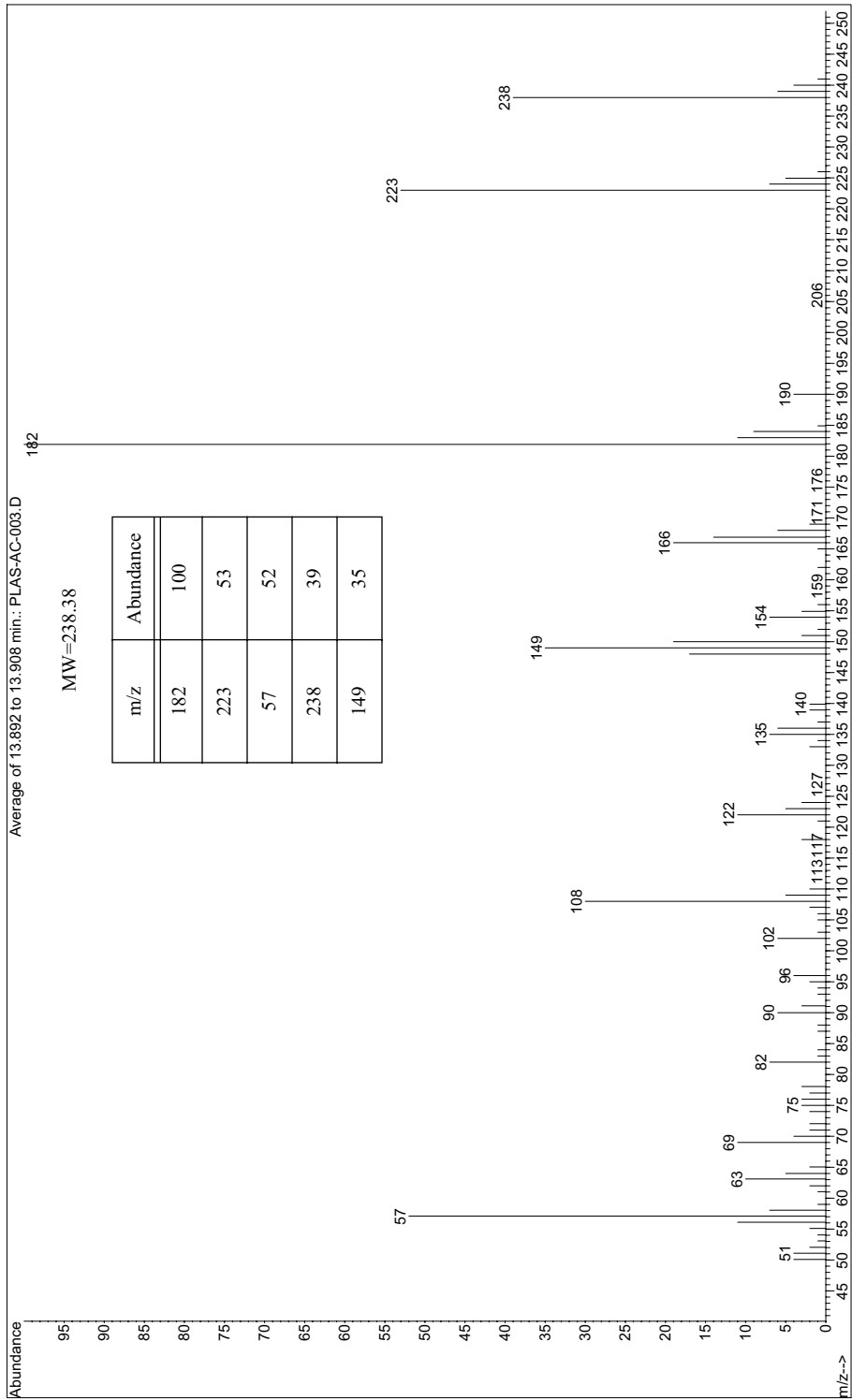
Point of Release

Due to the vulcanization process, finished rubber products contain only small amounts of TBBS or synthesis by-products (benzothiazole, 2-mercaptobenzothiazole, and 2-mercaptobenzothiazole disulfide). Release to the environment of these chemicals may occur during the use of rubber products. Fugacity model (Mackay level III) data suggest that it would mostly distribute to soil (if released to the air or soil compartments) and to water (if released to the water compartment).

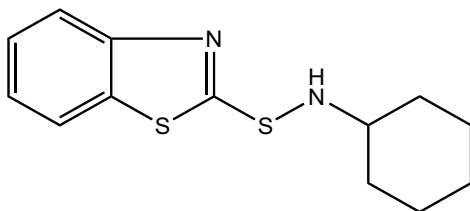
Toxicological Data

TBBS may be absorbed by the gastro-intestinal route, undergoing hydrolysis in vivo. Studies suggest that the hydrolysis products are toxic primarily to the liver and kidney. It was not found to be mutagenic in bacteria or in vitro mammalian gene mutation assays. It was not genotoxic in an in vivo mouse micronucleus assay. (LD50): >7940 mg/kg dermal [Rabbit]. It did induce chromosomal aberrations in mouse lymphoma cells in vitro with metabolic activation. Carcinogenicity not known.

Mass Spectrum for Accelerator BBTS - PLAS-AC-003



For Chromatogram See Appendix A - PLAS-AC-003 - page 440

Accelerator CBTS

CAS Number 95-33-0

RTECS Number DL6250000

Abbreviation CBTS

Formula $C_{13}H_{16}N_2S_2$

Molecular Weight 264.41

Chemical Name

N-(1,3-benzothiazol-2-ylsulfanyl)cyclohexanamine

Synonyms

N-cyclohexyl-2-benzothioazole sulfenamide

Brand Names & ManufacturersAccelerator CBTS
Santocure

Akrochem Corporation

Physical Properties**Appearance** White to tan powder**Melting Point** 102 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water 0.002	MeOH S	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application **Application, Regulatory & Environmental Information**

Delayed action sulfenamide accelerator for natural and synthetic rubbers. It provides better scorch resistance than thiazoles and can be accelerated by thiurams and dithiocarbamates to give shorter cure times. It can also be used as a retarder for ETU-cured polychloroprene and high thiuram cures.

Regulatory Information

Not FDA approved for food contact applications.

Environmental Impact

Not expected to be an environmental hazard.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

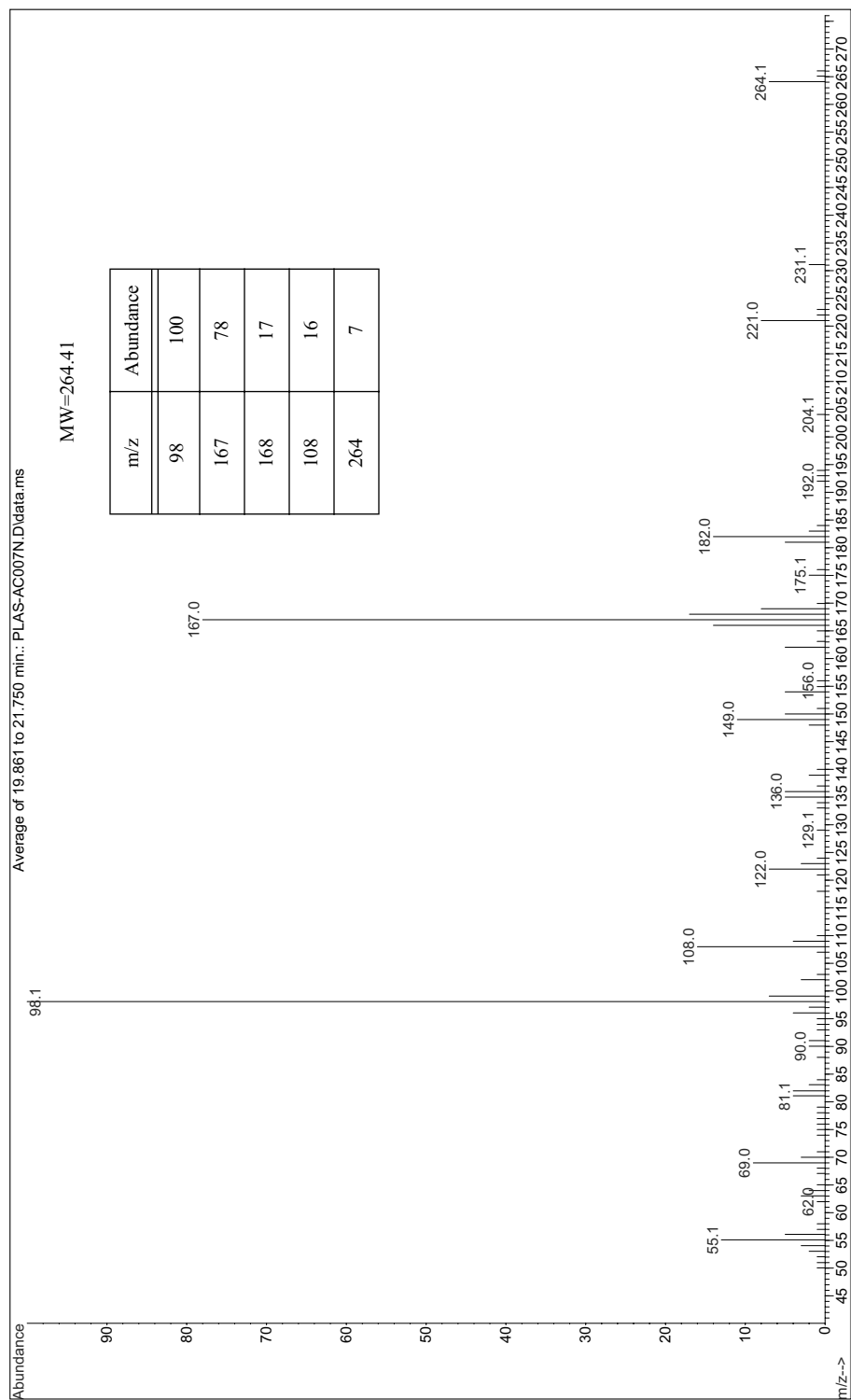
LD50 (oral): 5300 mg/kg [Rat]

LD50 (oral): >8000 mg/kg [Mouse]

LD50 (dermal): >7490 mg/kg [Rabbit]

Embryotoxic LD50 (intravenous): 32 mg/kg [Mice, Rodents]

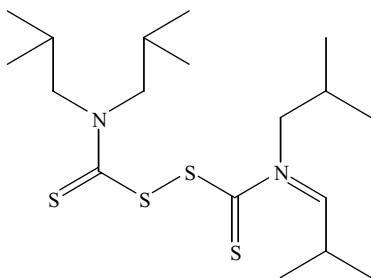
Mass Spectrum for Accelerator CBTS - PLAS-AC-007



For Chromatogram See Appendix A - PLAS-AC-007 - page 441

Cure-Rite® IBT

Noveon, Inc.

**CAS Number** 3064-73-1**RTECS Number** N/A**Abbreviation** TIBTD**Formula** C₁₈H₃₆N₂S₄**Molecular Weight** 408.76**Chemical Name**

tetraisobutylthiuram disulfide

Synonyms

tetra(isobutyl)thioperoxydicarbamic acid

Brand Names & Manufacturers

React-Rite® TIBTD

Resource Innovations, Inc.

Westco TIBTD

Western Reserve Chemical Corp.

Physical Properties**Appearance** Pale yellow to white powder**Melting Point** 70-73 °C**Boiling Point** Not available**Stability** Stable under normal conditions

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Used as an accelerator and vulcanizing agent in rubber (EPDM, SBR, Nitrile, and Natural). Especially useful when the formation of nitrosoamines is a concern.

Regulatory Information

FDA approved for use with rubber food-contact materials per 21CFR178.2010 and 178.3860.

Environmental Impact

Due to its low solubility in water and therefore the non-availability to species, this product is not expected to be toxic to aquatic organisms. Estimated log Kow value of 3.4 indicates a low to moderate potential to bioaccumulate.

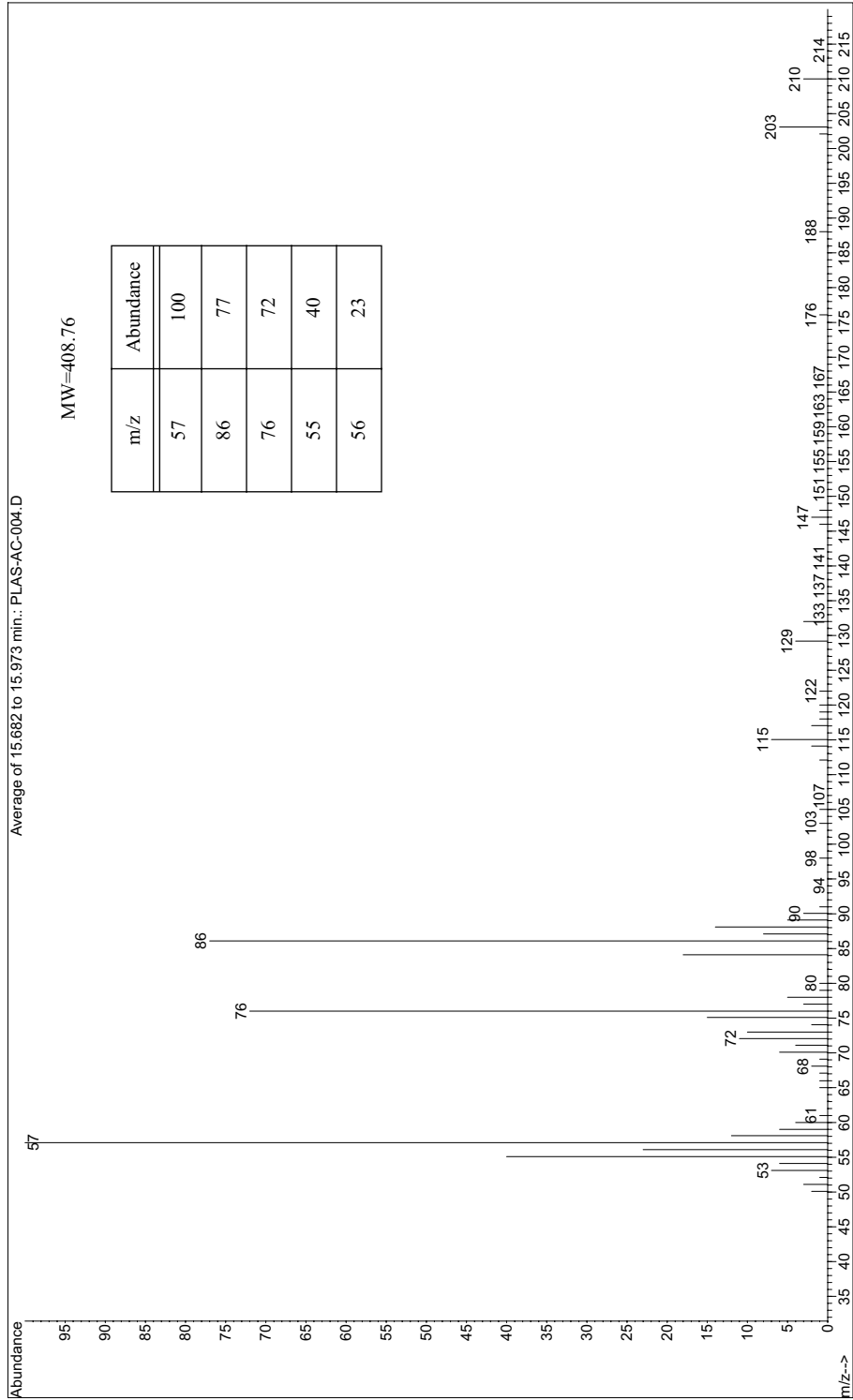
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

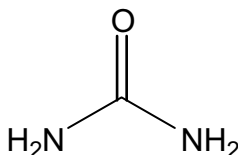
Mass Spectrum for Cure-Rite® IBT - PLAS-AC-004



For Chromatogram See Appendix A - PLAS-AC-004 - page 447

Activator OT Urea

Akrochem Corporation

**CAS Number** 57-13-6**RTECS Number** YR6250000**Abbreviation** Not Identified**Formula** CH₄N₂O**Molecular Weight** 60.07**Chemical Name**

urea

Synonyms

carbonyl diamide; carbamide; isourea

Brand Names & Manufacturers

Supercel 3000

Varioform II

Physical Properties

Appearance	White solid					
Melting Point	133-135 °C			Boiling Point	Decomposes 135 °C	
Stability	Decomposes at 135 °C (MP)					
Solubility (g/100mL 20 °C)	Water >80	MeOH ~16	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application Urea is used in the manufacture of urea-formaldehyde plastics, adhesives, polymers, synthetic fibers, dyes, etc.

Regulatory Information

FDA approved 1998 for the following applications: in the manufacture of resin and polymer-based coatings in contact with food, 21CFR175.300; in the manufacture of cellophane for packaging food, 21CFR177.1200. EU (1990) determined urea acceptable for use in plastic materials in contact with foodstuffs. In 1993, a joint FAO/WHO Committee on food additives determined 3% urea in chewing gum is not toxic.

Environmental Impact

Although urea has generally low ecotoxicity to organisms, its well-documented indirect and long-term effects to the ecosystems, e.g., eutrophication, groundwater pollution, soil acidification, and ammonia emissions to air, should be considered. When released to soil, this material will hydrolyze into ammonium in a matter of days to several weeks. This material is not anticipated to bioaccumulate — it has a BCF <100.

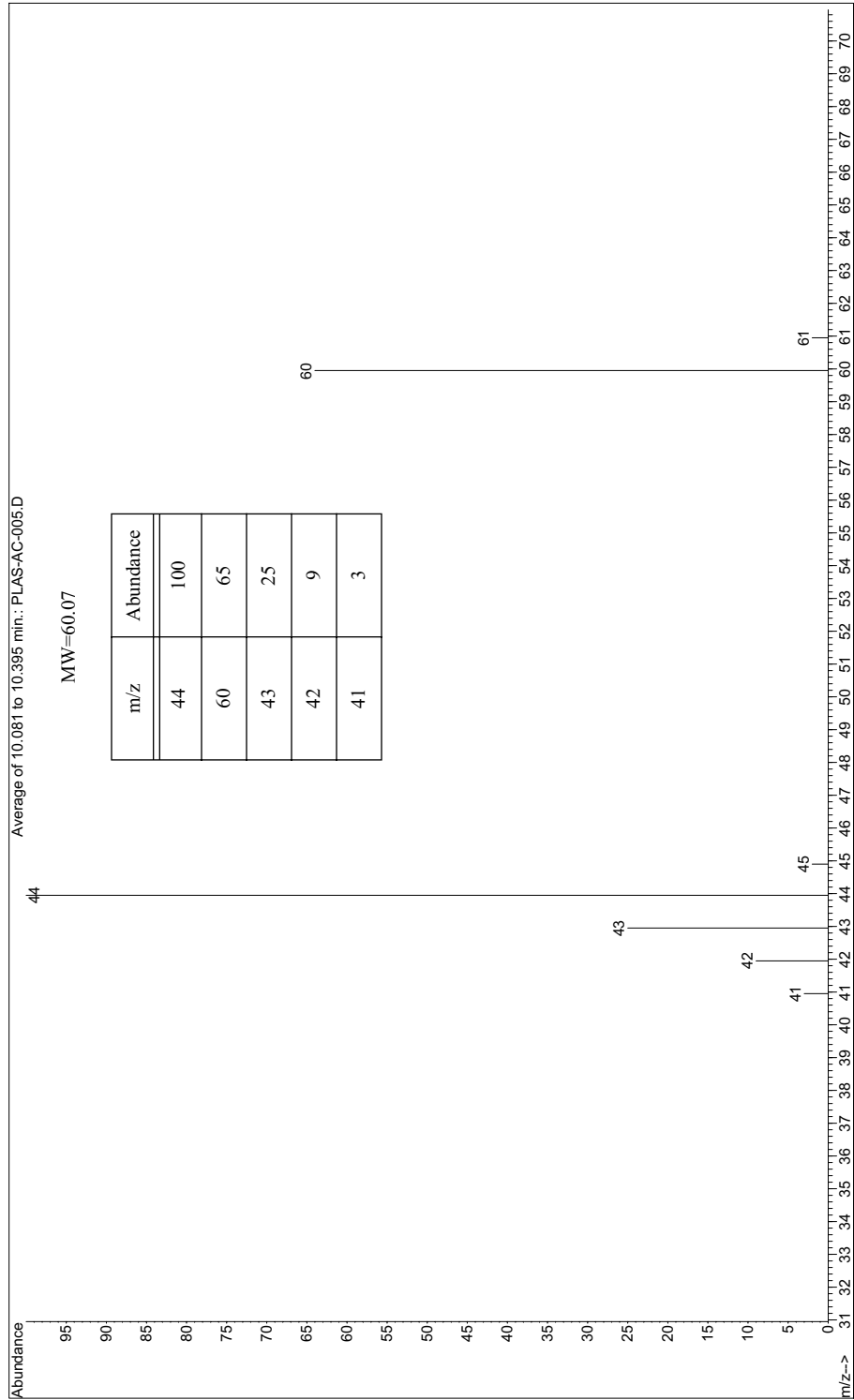
Point of Release

Occupational and environmental exposure during production is possible due to accidental process breakdown and disorders in reactor operations, pumping cycles, evaporation, and crystallization processes; in maintenance, loading and unloading operations. Potential occupational exposure occurs via inhalation of aerosols from urea melt and hot saturated solutions, splashed to skin or eyes, or inhalation of dust.

Toxicological Data

No documented toxic effects at low doses. Chronic exposure is carcinogenic and mutagenic: 821 g/kg [Rat] and 394 g/kg [Mouse] for one year results in lymphomas and Hodgkin's disease. Long-term toxicity: High doses affect cholinergic and bioenergetic processes and modify CNS structure. Acute oral toxicity (LD50): 14.3 g/kg BW [Rat], 11 g/kg [Mouse].

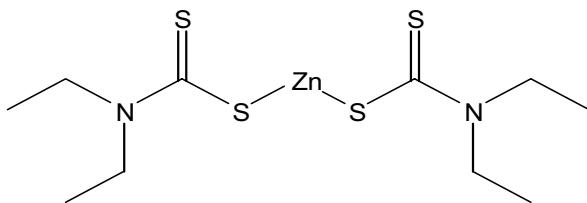
Mass Spectrum for Activator OT Urea - PLAS-AC-005



For Chromatogram See Appendix A - PLAS-AC-005 - page 446

Accelerator EZ & EZ-SP

Akrochem Corporation

**CAS Number** 14324-55-1**RTECS Number** ZH0350000**Abbreviation** DEDTZ/ZDEC**Formula** $C_{10}H_{20}N_2S_4 \cdot Zn$ **Molecular Weight** 361.93**Chemical Name**

zinc diethyldithiocarbamate

Synonyms

bis(diethyldithiocarbamato)zinc; diethyldithiocarbamic acid, zinc salt; ethyl zimate

Brand Names & Manufacturers

Ethasan	Solutia, Inc.
Perkacit® ZDEC	Akzo Nobel Chemicals B.V.
Soxinol® EZ	Sumitomo Chemical Co., Ltd.
Vulcacure	Alco Oil and Chemical Corp.

Physical Properties

Appearance	White powder					
Melting Point	178-181 °C			Boiling Point	Not available	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone S	CH₂Cl₂ S	Hexane U

Application **Application, Regulatory & Environmental Information**

ZDEC is used in the following applications: as a fast primary or secondary vulcanization accelerator in NR, SBR, IIR, EPDM and for natural and synthetic latex; a stabilizer in butyl, butadiene, and urethane rubbers; an antioxidant in rubber-based adhesive systems; a stabilizer in cement; a heat stabilizer for polyethylene.

Regulatory Information

FDA approved 1998 for use as an accelerator in the manufacture of rubber material (up to 1.5% of weight of rubber) intended for use in all stages of production, processing, packaging, and transport of food: 21CFR177.2600. Regulated for use under 21CFR175.105 for components of adhesives.

Environmental Impact

Ecological impact not determined. Similar compounds show low to moderate biodegradability, but rapid hydrolysis under acidic conditions. Similar compounds are also determined to have low bioaccumulation potential and environmental persistence: 96 hour LC50 0.23 mg/L [Rainbow Trout], 0.40 mg/L [Bluegill Sunfish], 0.26 mg/L [Fathead Minnow], 48 hour EC50 0.44 mg/L [Daphnia Magna].

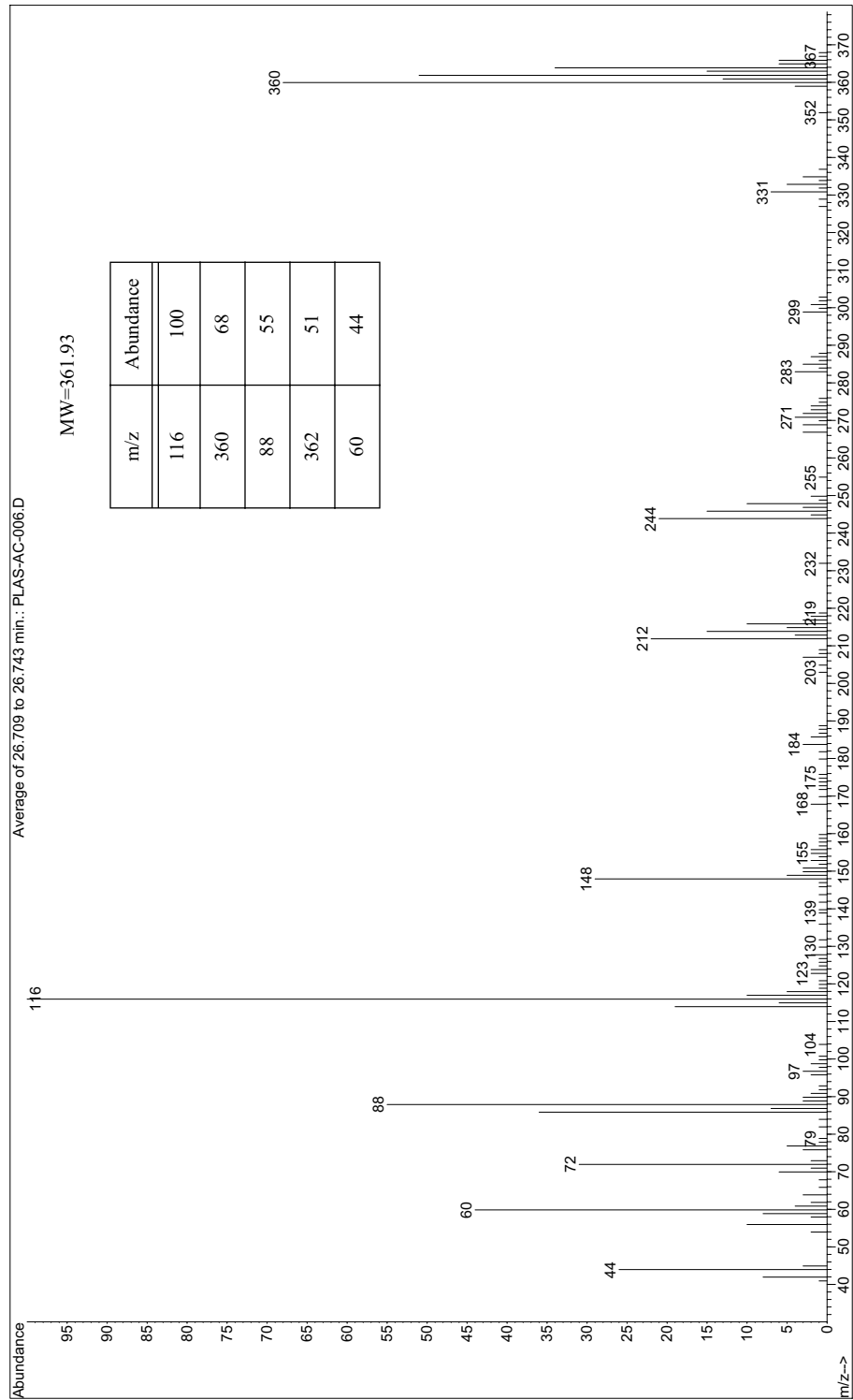
Point of Release

Migration of ZDEC into water after 3 days exposure at 20 °C is 0.6 mg/L.

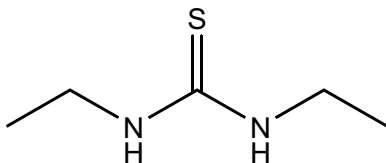
Toxicological Data

Not listed as a suspected carcinogen by NTP, IARC, or OSHA. Reactions with nitrosylating agents during vulcanization may yield suspected carcinogens such as nitrosamines. Studies of rats and mice gavaged with ZDEC yield no genotoxic or teratogenic effects. Long-term exposure to large doses may have neurodegenerative effects in addition to altering hydrolytic enzymes in the human brain. Acute oral (LD50): 3530 mg/kg [Rat]. Acute dermal (LD50): >3160 mg/kg [Rabbit].

Mass Spectrum for Accelerator EZ & EZ-SP - PLAS-AC-006



For Chromatogram See Appendix A - PLAS-AC-006 - page 443

N, N'-Diethylthiourea

CAS Number 105-55-5

RTECS Number YS9800000

Abbreviation DETU

Formula C₅H₁₂N₂S

Molecular Weight 132.23

Chemical Name

1,3-diethylthiourea

Synonyms

1,3-diethyl-2-thiourea; N,N'-diethylthiocarbamide

Brand Names & Manufacturers

Accelerator DETU

Akrochem Corporation

Thiate[®] H

RT Vanderbilt

Westco DETU

Western Reserve Chemical

Pennzone E

Physical Properties**Appearance** White semi-transparent crystals**Melting Point** 68-71 °C**Boiling Point** 169 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water 3.8	MeOH S	EtOH S	Acetone S	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Accelerator for mercaptan-modified chloroprene rubber. Stabilizer for natural, nitrile-butadiene, styrene-butadiene, and chloroprene rubbers. Found in adhesives, animal repellent, cements, condoms, cosmetic applicators, disinfectants, fungicides, gloves, leather shoes, rubber in undergarments, tires and tubes, soaps and shampoos.

Regulatory Information

Regulated for use under 21 CFR §177.2600 Rubber Articles Intended for Repeated Use in Food Contact.

Environmental Impact

If released to soil, biodegradation of N,N-diethylthiourea may be an important removal process. Because of the estimated low K_{oc} value in soil, N,N-diethylthiourea may rapidly leach in soil. The volatilization of N,N-diethylthiourea from moist soil is not expected to be an important removal process. Neither photolysis nor hydrolysis are expected to be important in water. BCF = 2.

Point of Release

The release of N,N-diethylthiourea in the environment is expected to occur during waste disposal from its production and use.

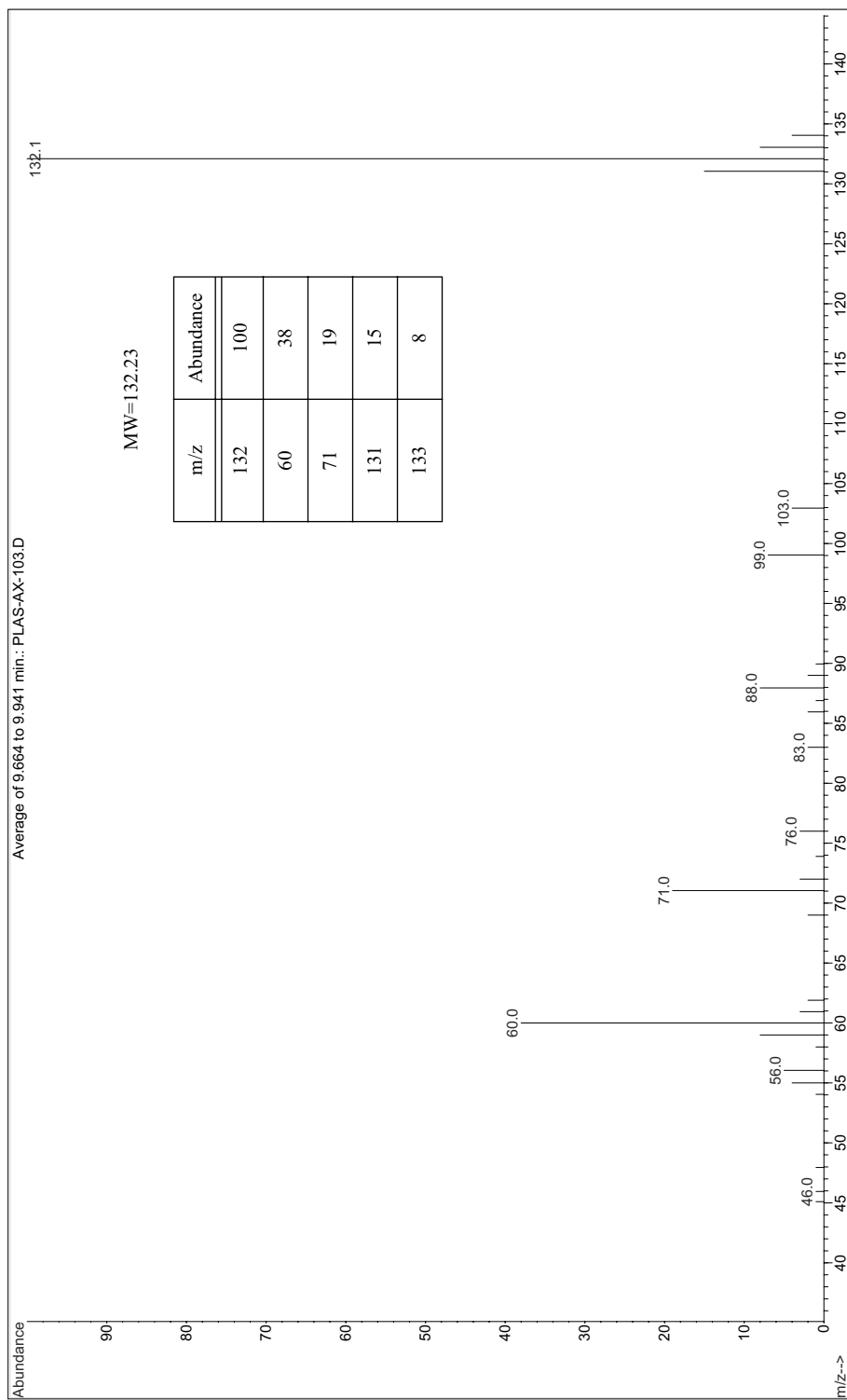
Toxicological DataOral (LD₅₀): = 316 mg/kg [Rat]

Oral (TDLo): = 11 gm/kg/2Y-C [Rat]

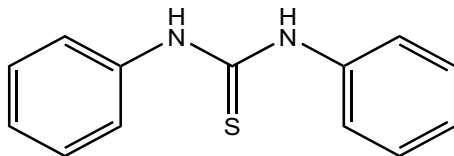
Tumorigenic - Carcinogenic by RTECS criteria; Endocrine - thyroid tumors Mutation in mammalian somatic cells (mouse lymphocyte) = 1500 mg/L

Bacteria: Phytobacterium phosphoreum: 761.0 mg/L; 15 minute Microtox test: No data available.

Mass Spectrum for N, N'-Diethylthiourea - PLAS-AX-103



For Chromatogram See Appendix A - PLAS-AX-103 - page 444

1,3-Diphenyl-2-thiourea

CAS Number 102-08-9

RTECS Number FE1225000

Abbreviation DPTU

Formula C₁₃H₁₂N₂S

Molecular Weight 228.31

Chemical Name

1,3-di(phenyl)thiourea

Synonyms

N,N'-diphenylthiocarbamide

Brand Names & Manufacturers

Accelerator Thio #1

Akrochem

Vulkacit CA

Lanxess

Westco DPTU

Western Reserve Chemical

Physical Properties**Appearance** White powder**Melting Point** 152-155 °C**Boiling Point** 348-350 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH S	EtOH S	Acetone S	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application**

Used as a primary or secondary vulcanization accelerator.

Regulatory Information

Regulated for use under the following sections of 21 CFR:

§177.2600 Rubber Articles Intended for Repeated Use in Food Contact

§175.105 Components of Adhesives

Environmental Impact

Level III Fugacity Model:	Mass Amount (%)	Half-Life (h)	Emissions (kg/h)	
Air	0.0975	3.01	1000	
Water	17	900	1000	
Soil	82.2	1.8e+003	1000	
Sediment	0.626	8.1e+003	0	Persistence Time: 1.17e+003 h

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

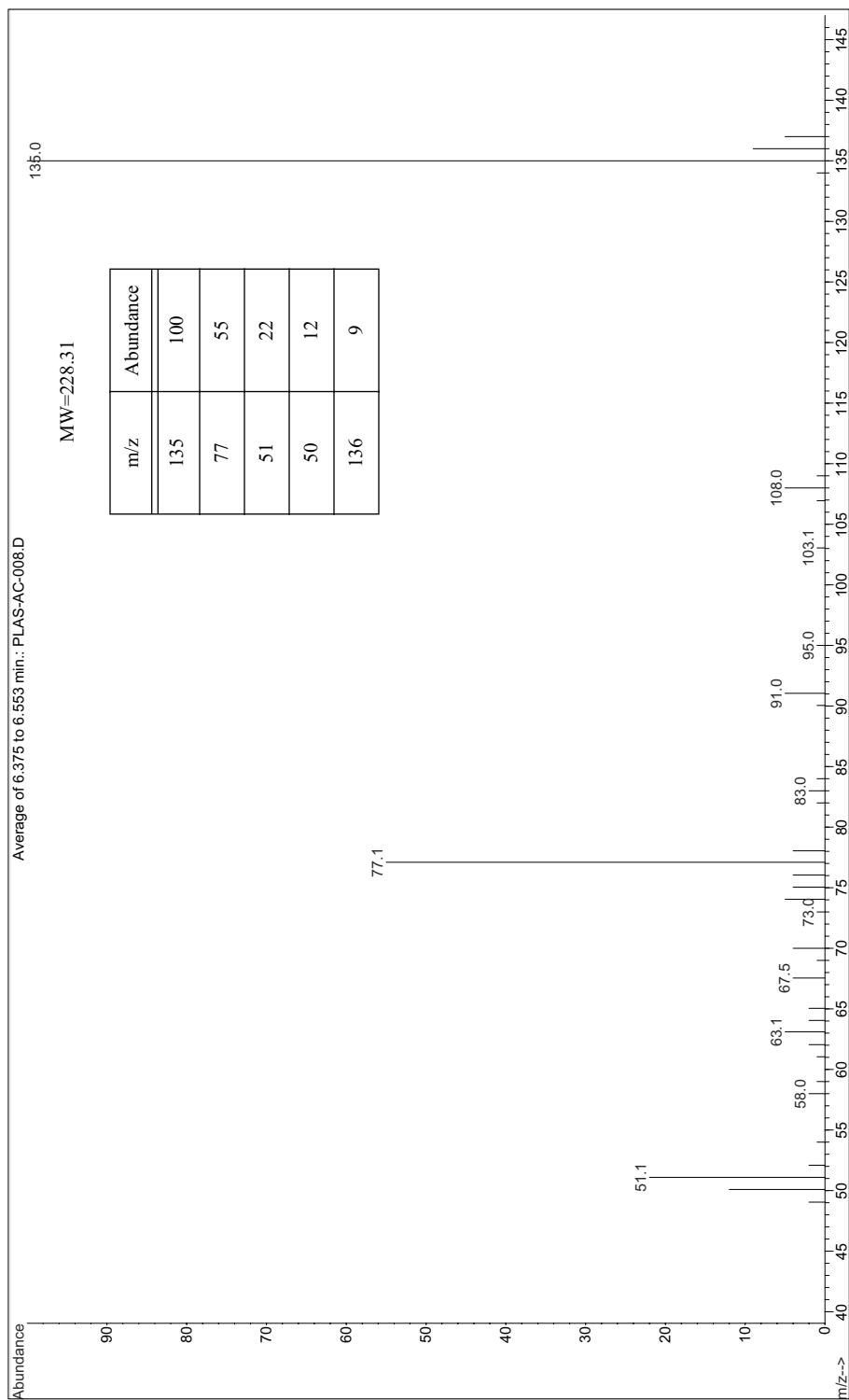
Toxicological Data

Oral (LD50): 50 mg/kg [Rat]

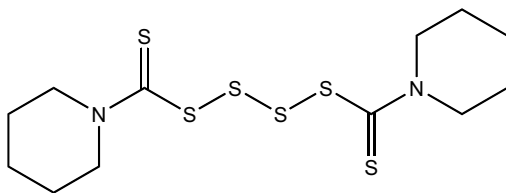
Intraperitoneal (LD50): 1 gm/kg [Rat]

Intraperitoneal (LD50): 500 mg/kg [Mouse]

Mass Spectrum for 1,3-Diphenyl-2-thiourea - PLAS-AC-008



For Chromatogram See Appendix A - PLAS-AC-008 - page 449

Dipentamethylenethiuram Tetrasulfide


CAS Number 120-54-7

RTECS Number TN4221000

Abbreviation DPTT

Formula $C_{12}H_{20}N_2S_6$

Molecular Weight 384.70

Chemical Name**Synonyms**

1,1'-(tetrathiodicarbonothioyl)-bis-piperidine

Brand Names & Manufacturers
Westco DPTT
Tetrone A

Western Reserve Chemical

Physical Properties
Appearance Light yellow to gray powder**Melting Point** 115 °C**Boiling Point** 510 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone S	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information
Application This compound is used as primary or secondary accelerator or sulfur donor for both natural rubber and synthetic.**Regulatory Information**

Regulated for use in articles in contact with food as specified under FDA §175.105, §175.300, §177.1210 (indirect food contact).

Environmental Impact

Contains no hazardous air pollutants or ozone depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

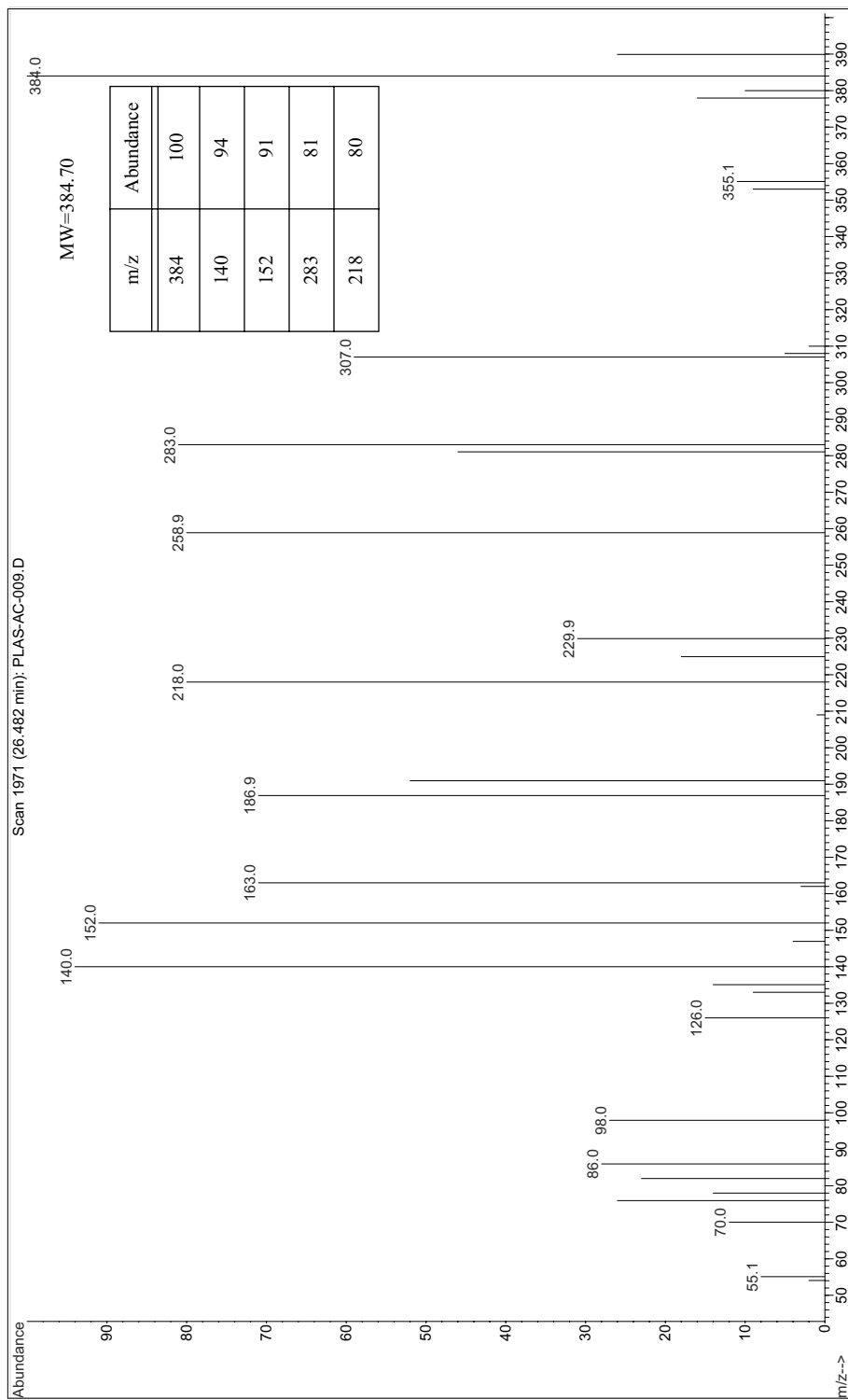
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

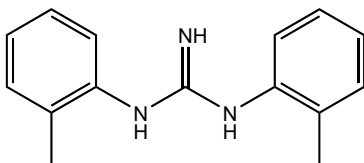
Toxicological Data

Oral (LD50): > 2000 mg/kg [Rat]

Mass Spectrum for Dipentamethylenethiuram Tetrasulfide - PLAS-AC-009



For Chromatogram See Appendix A - PLAS-AC-009 - page 450

1,3-Di-o-tolylguanidine

CAS Number 97-39-2

RTECS Number MF1400000

Abbreviation DOTG

Formula C₁₅H₁₇N₃

Molecular Weight 239.32

Chemical Name

1,2-bis(2-methylphenyl)guanidine

Synonyms

Di-o-tolylguanidine

Brand Names & Manufacturers

Accelerator DOTG	Timeliall
DOTG	Western Reserve Chemical
Sovchem® DOTG	Sovereign Chemical Company
VANAX® DOTG	RT Vanderbilt

Physical Properties

Appearance	White powder					
Melting Point	175 - 178 °C			Boiling Point	N/A	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH S	EtOH S	Acetone S	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application Seldom used alone, commonly used with thiazoles, thiurams, dithiocarbamates, and sulfenamides to promote its activity as an accelerant. Mainly used in processing thick rubber products, tread rubber, breaker rubber, and rubber roll cover.

Regulatory Information

Regulated for use under the following sections of 21 CFR:
 §177.2600 Rubber Articles Intended for Repeated Use in Food Contact
 §175.105 Components of Adhesives
 §178.3120 Animal Glue

Environmental Impact

Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

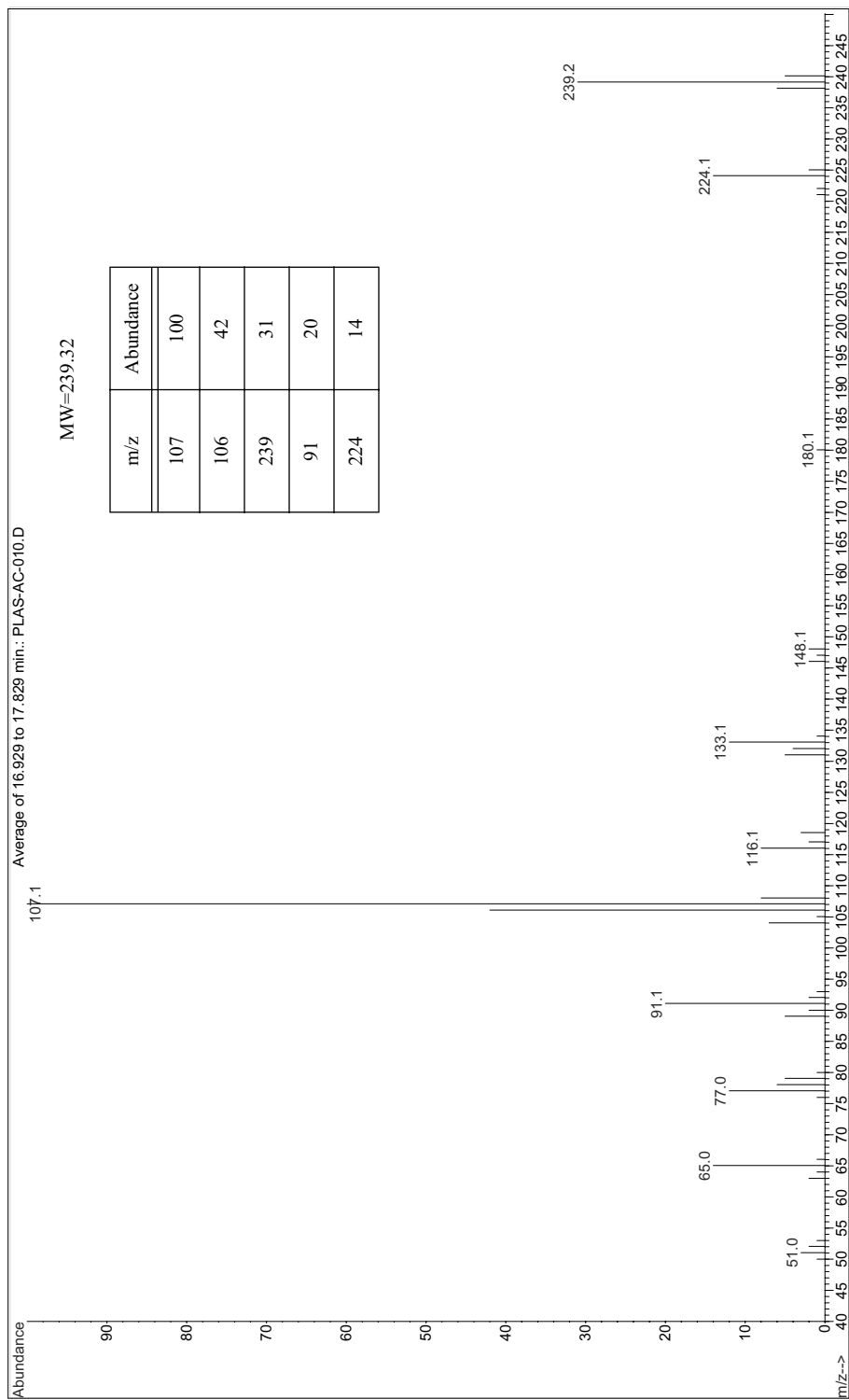
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

LD50 Oral - Mammal - 120 mg/kg
 LD50 Oral Rat 56 mg/kg

Mass Spectrum for 1,3-Di-o-tolylguanidine - PLAS-AC-010



For Chromatogram See Appendix A - PLAS-AC-010 - page 451

Stabilizers

Stabilizers include a wide range of organic and inorganic compounds that are compounded into polymeric materials to inhibit degradation due to various environmental exposures. Inorganics include acid scavengers and materials that inhibit water penetration, for example. These are beyond the scope of this Handbook.

It is important to note that while stabilizers can be divided into categories based on functionality, degradation of many polymers often occurs through sequential processes. For example, ultraviolet radiation will typically split bonds in many types of polymers. The broken chain ends are made reactive as a result and will typically react with ambient oxygen. Thus, ultraviolet energy indirectly causes oxidation. Protection of a polymer exposed to strong sunlight, for example, may be sufficiently protected with an ultraviolet inhibitor in the absence of an antioxidant; however, an antioxidant alone would not prevent polymer degradation. While oxidation may not occur, chain scission would progress, resulting in crazing and cracking of the polymer.

Organic stabilizers fall into several general categories, with some specialized types that are designed for plastics in technical applications. The largest class of stabilizers includes antioxidants. These are addressed in a dedicated chapter of this Handbook.

Antiozonants

These materials are added to plastics to slow the deterioration of the finished product that occurs from exposure to ozone. They typically function by migrating to the surface of the product and then create an ozone-inhibiting barrier layer at the surface. The most effective ozone inhibitors include trimethylquinolines and phenylenediamines. Their functionality is achieved through interference with ozone-induced free radical reactions with the host polymer.

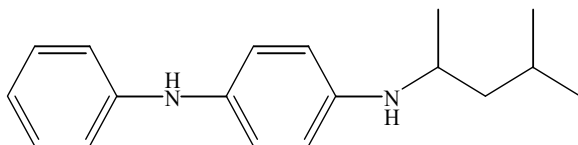
Ultraviolet Inhibitors

Ultraviolet (UV) radiation from solar exposure and prolonged exposure to artificial UV sources can be very destructive to polymers used in vinyl siding, windows, doors, outdoor furniture, and appliances, for example. UV inhibitors help prevent discoloration, cracking, embrittlement, “chalking”, and loss of physical properties in these products that may occur upon exposure to UV.

The most common UV absorbers used commercially are hindered amine light stabilizers, which can also function as antioxidants in some plastics. Other UV absorbers include benzotriazoles and benzophenones, salicylate esters, cyanoacrylates, malonates, and benzilidenes. Factors such as the type of polymeric resin, type and level of pigments being used, and the presence of crosslinking compounds and catalysts govern the selection of UV absorber to be used.

Santoflex® 6PPD

Flexsys



CAS Number 793-24-6
RTECS Number N/A
Abbreviation Not Identified

Formula C₁₈H₂₄N₂
Molecular Weight 268.40

Chemical Name

N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine

Synonyms

N/A

Brand Names & Manufacturers

Santoflex 6PPD

Flexsys

Physical Properties

Appearance	Off-white to dark-brown pastilles					
Melting Point	46-51 °C			Boiling Point 227 °C		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH >80	Acetone >80	CH₂Cl₂ U	Hexane U

Application**Application, Regulatory & Environmental Information**

Provides antiozonant and antioxidant properties with high temperature, fatigue, and flex resistance to rubber compounds. Used in pneumatic tire components, solid tires, belts, hoses, cables, automotive mounts, bushings, and general mechanical products that are exposed to continuous and intermittent dynamic operating conditions that require protection from ozonation.

Regulatory Information

Santoflex 6PPD is not approved for use in FDA food contact applications.

Environmental Impact

Octanol/Water Coefficient: 59000 ± 34000 (Calculated). Log P = 4.68. Chemical Fate Information: Bioconcentration Factor = 490 (calculated). Other Information: Aerobic Biodegradation: 50% after 2.9 hours. Rapid degradation via hydrolysis: 93% after 24 hours at pH 7.0 and 25°C. Tests indicate this material will not bioaccumulate or persist in the environment.

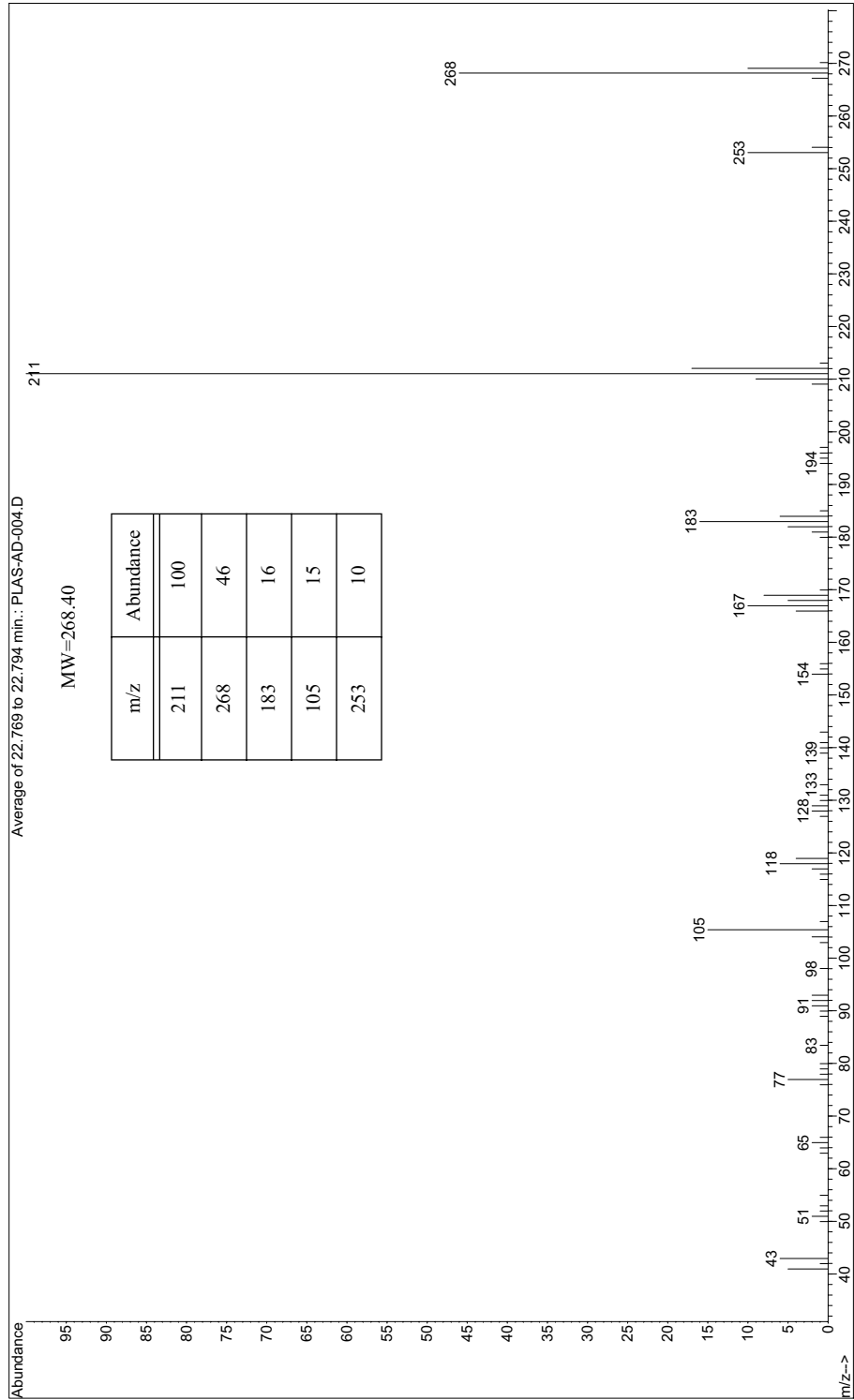
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): 3580 mg/kg [Rat]; acute dermal (LD50): >7940 mg/kg [Rabbit]. Not listed as a carcinogen or a suspected carcinogen by NTP, IARC, or OSHA.

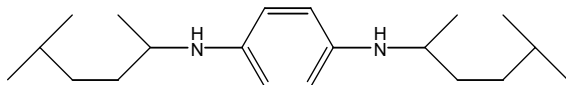
Mass Spectrum for Santoflex® 6PPD - PLAS-AD-004



For Chromatogram See Appendix A - PLAS-AD-004 - page 448

Santoflex® 77PD

Solutia Inc.

**CAS Number** 3081-14-9**RTECS Number** SS8400000**Abbreviation** Not Identified**Formula** C₂₀H₃₀N₂**Molecular Weight** 304.58**Chemical Name**

N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine

Synonyms

N,N'-di(1,4-dimethylpentyl)-p-phenylenediamine

Brand Names & Manufacturers

Santoflex 77PD

Solutia Inc.

Physical Properties**Appearance** Dark-red oily liquid**Melting Point** -36 °C**Boiling Point** 183 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH >80	Acetone >80	CH₂Cl₂ U	Hexane U
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Application**Application, Regulatory & Environmental Information**

Santoflex 77PD is used as an antiozonant in natural and synthetic elastomer compounds that can tolerate discoloration (it will discolor compounds and cause severe contact and migration staining). It also protects against catalytic degradation by copper and other heavy metals.

Regulatory Information

Santoflex 77PD is regulated for use in articles in contact with food as specified under BgVV XXI, Category 4 (Germany). Santoflex 77PD is not regulated for use in FDA food contact applications.

Environmental Impact

Acute Fish Toxicity: (LC50 96 hour): 32 mg/L [Rainbow Trout], 182 mg/L [Bluegill Sunfish], 0.28 mg/L [Fathead Minnow]. Bioaccumulation, potential, 5.34 log Pow. This product rapidly degrades via hydrolysis up to 97% after 24 hours at pH 7.0 at 25°C. Tests indicate this material will not bioaccumulate or persist in the environment.

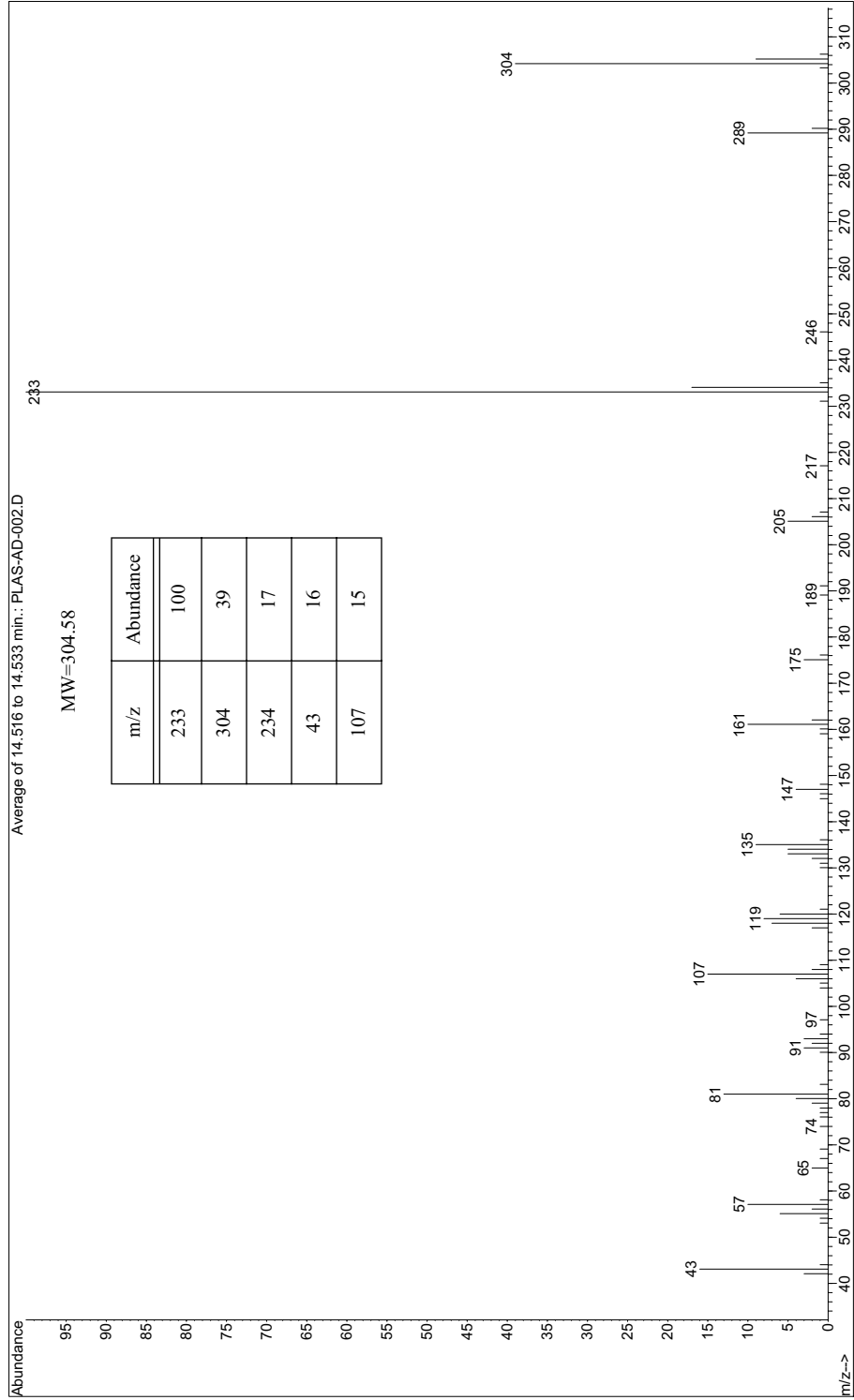
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

(LD50): 750 mg/kg–1.6 g/kg BW [Rat], 0.8 g/kg BW [Mouse]. This material or its emissions may cause an allergic or sensitization reaction and thereby aggravate systemic disease such as liver disorders. This compound is not listed as a carcinogen or suspected carcinogen by NTP, IARC, or OSHA.

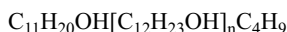
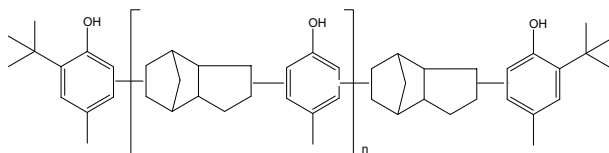
Mass Spectrum for Santoflex® 77PD - PLAS-AD-002



For Chromatogram See Appendix A - PLAS-AD-002 - page 452

Lowinox® CPL

Chemtura Corporation

**CAS Number** 68610-51-5**RTECS Number** N/A**Abbreviation** Not Identified**Formula** See below structure**Molecular Weight** 600–700**Chemical Name**

butylated reaction product of p-cresol and dicyclopentadiene

Synonyms

poly (dicyclopentadiene-co-p-cresol); polymeric sterically hindered phenol

Brand Names & Manufacturers

Antioxidant 12

Akrochem Corporation

WingStay® L

Eliokem

Vanox® L

R.T. Vanderbilt Company, Inc.

Physical Properties**Appearance** Yellow-brown powder or pellets**Melting Point** >105 °C**Boiling Point** Not available**Stability** Stable under normal conditions.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	10-40	10-40	5-40	U	<0.1

Application, Regulatory & Environmental Information

Application Applications include in-process stabilization of polymers as well as use in manufactured goods such as elastic thread, carpet backing, foam rubber mattresses, household and surgical gloves, medical products, baby bottle teats, bath mats, hot water bottles, automotive components, household appliances (gaskets, liners, parts, housing, etc.), electronic appliance housings, and paper coatings.

Regulatory Information

This product is approved for use by the FDA in a number of food-contact applications as an Indirect Food Additive, including 21CFR175.105 (Components of Adhesives); 21CFR175.125 (Pressure-Sensitive Adhesives); 21CFR177.2600 (Rubber Articles - Antioxidants); and 21CFR178.2010 (Antioxidants and/or Stabilizers for Polymers).

Environmental Impact

This product is not biodegradable and has a high potential to bioaccumulate based on an estimated log Kow value greater than 9. It is not expected to be toxic to fish due to its low water solubility.

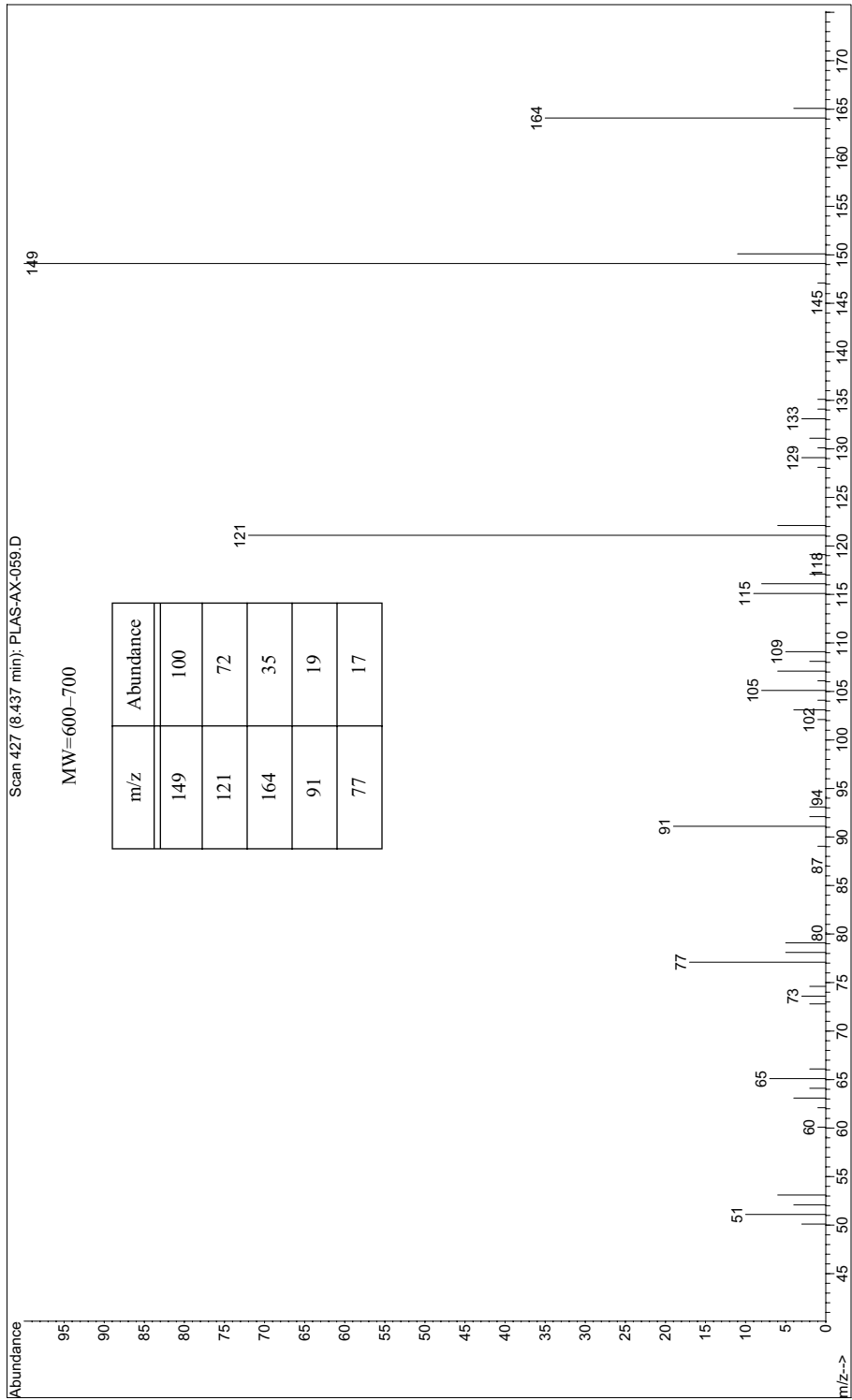
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

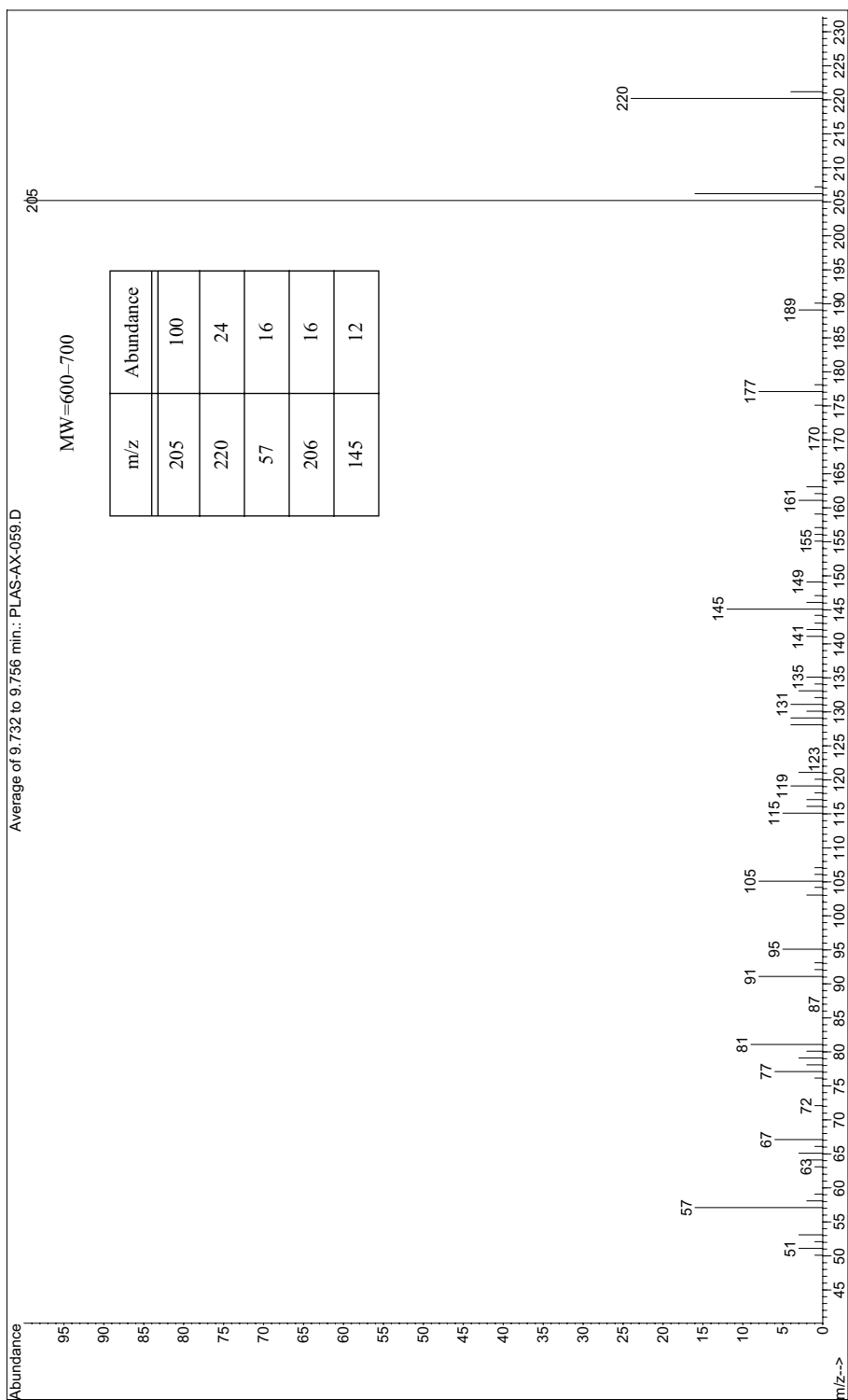
Toxicological Data

Acute oral toxicity (LD50): >4000 mg/kg [Rat], acute dermal toxicity (LD50): >5010 mg/kg [Rabbit], acute inhalation (LC50) >165 mg/kg [Rat], not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectrum for Lowinox® CPL - PLAS-AX-059

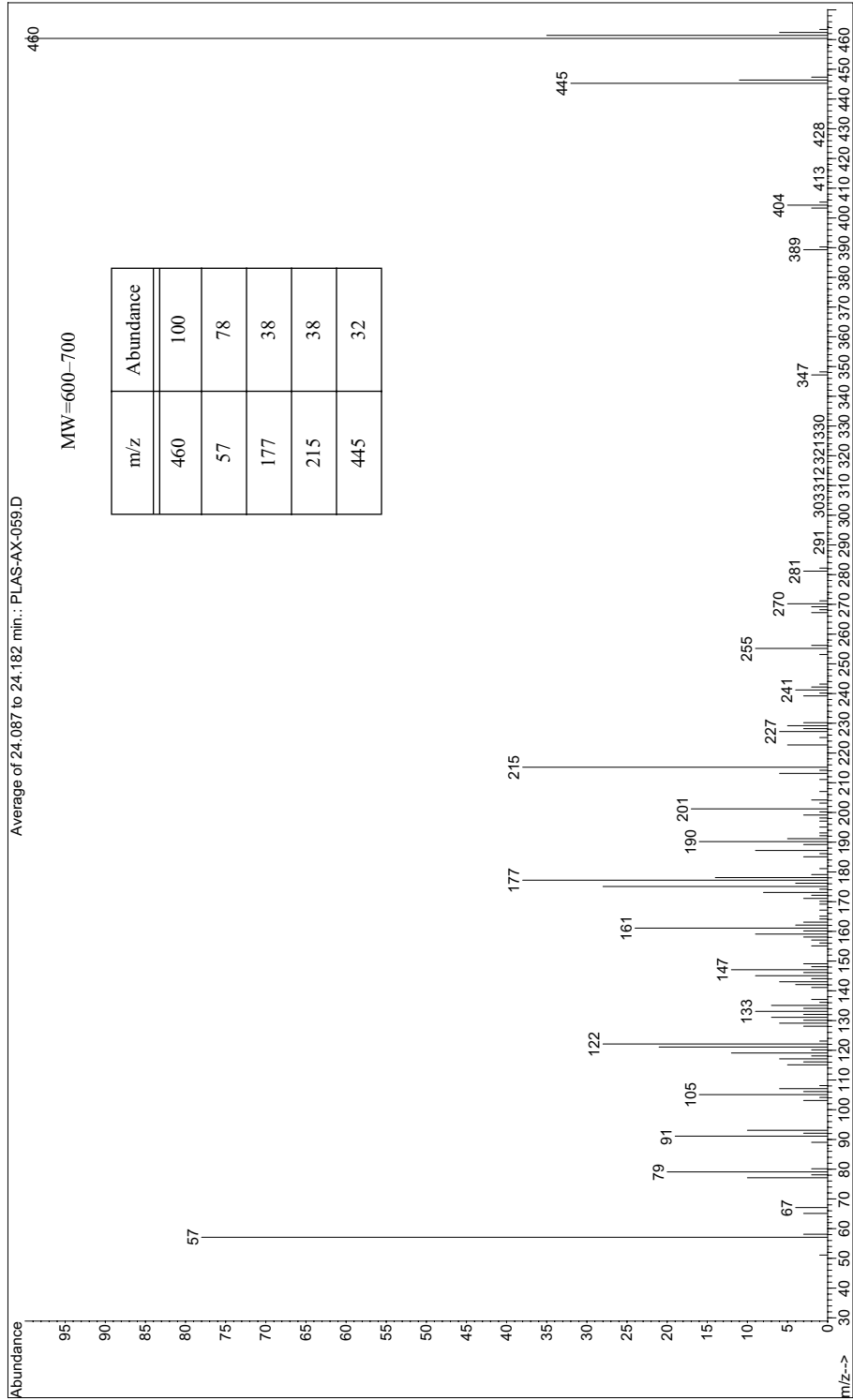


For Chromatogram See Appendix A - PLAS-AX-059 - page 453

Mass Spectrum for Lowinox[®] CPL - PLAS-AX-059

For Chromatogram See Appendix A - PLAS-AX-059 - page 453

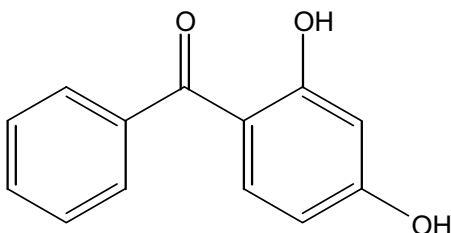
Mass Spectrum for Lowinox® CPL - PLAS-AX-059



For Chromatogram See Appendix A - PLAS-AX-059 - page 453

Uvinul® 3000

BASF Corporation



CAS Number 131-56-6

RTECS Number DJ0700000

Abbreviation Not Identified

Formula C₁₃H₁₀O₃

Molecular Weight 214.22

Chemical Name

2,4-dihydroxybenzophenone

Synonyms

(2,4-dihydroxyphenyl)phenylmethanone; benzophenone-1

Brand Names & Manufacturers

Dansorb® 240

Dannier

Lowilite® 24

Chemtura Corporation

Magnolol

Atkin Chemicals

Physical Properties**Appearance** Off-white powder**Melting Point** 144 °C**Boiling Point** 194 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	34	40	70.9	U	1.0

Application**Application, Regulatory & Environmental Information**

This product is an ultraviolet light absorber for use in polystyrene, unsaturated polyesters, coatings, varnishes, lacquers, and coatings based on epoxy or phenolic alkyds. It is also used in pressure sensitive adhesives, polymethylacrylate (film or sheeting), thermoplastic rubbers, polyisoprene latex, and alcohol-based cosmetics.

Regulatory Information

This product is not approved by the FDA for food contact applications.

Environmental Impact

Readily biodegradable and is not expected to bioaccumulate based on a log Pow value of 2.96 and its insolubility in water.

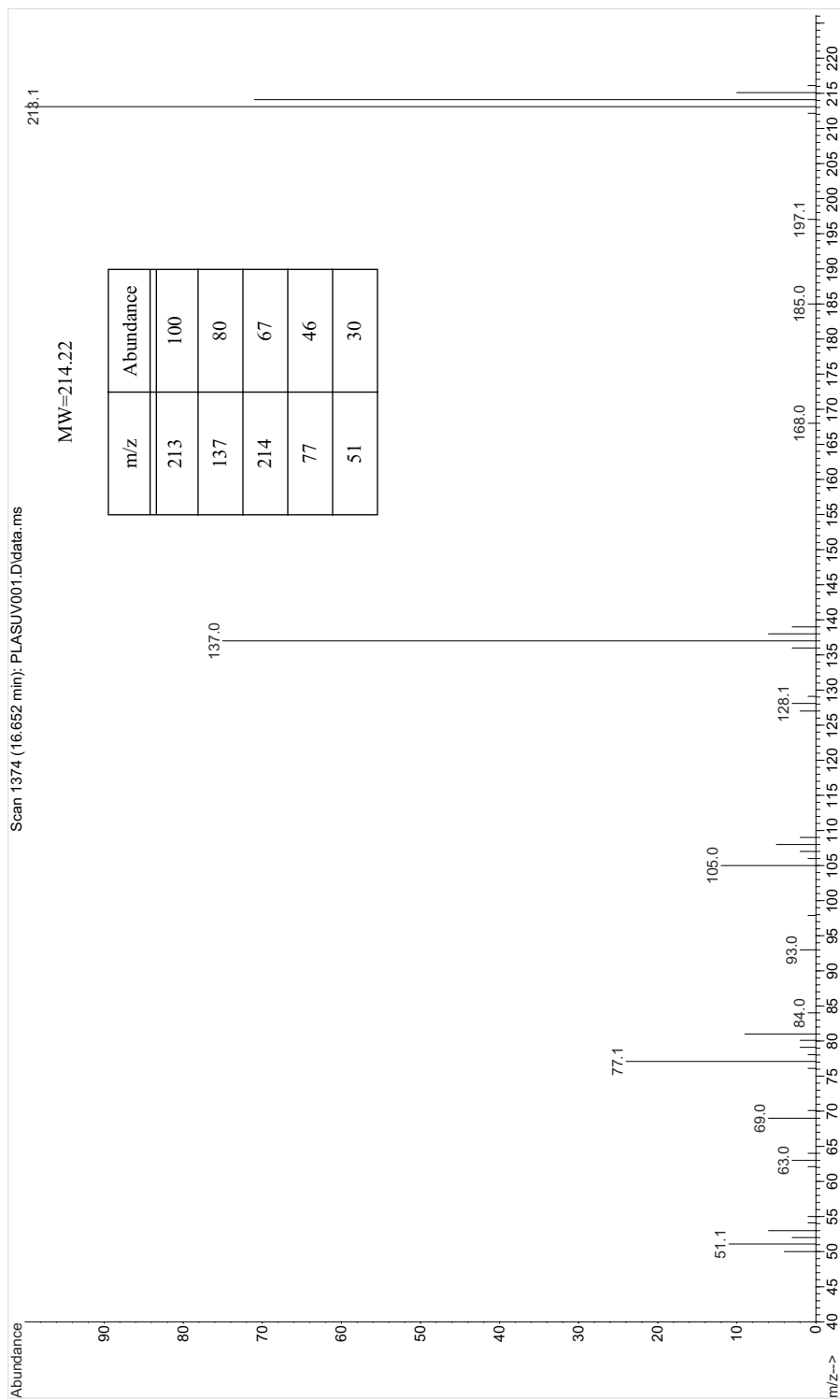
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

May cause chronic liver, kidney, and blood effects based on animal data. Acute oral (LD50): >2000 mg/kg [Rat], 2500 mg/kg [Mouse]. Carcinogenicity: Not listed by ACGIH, IARC, NIOSH, NTP, or OSHA.

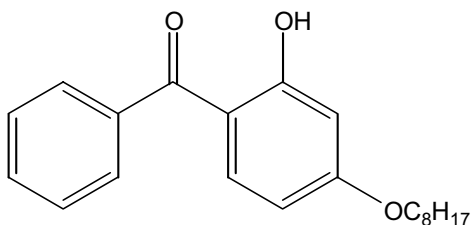
Mass Spectrum for Uvinul® 3000 - PLAS-UV-001



For Chromatogram See Appendix A - PLAS-UV-001 - page 454

Uvinul® 3008

BASF Corporation



CAS Number 1843-05-6
RTECS Number DJ1595000
Abbreviation Not Identified

Formula C₂₁H₂₆O₃
Molecular Weight 326.43

Chemical Name

2-hydroxy-4-octyloxybenzophenone

Synonyms

octabenzene; (2-hydroxy-4-(octyloxy)phenyl)phenylmethanone

Brand Names & Manufacturers

Chimassorb® 81	Ciba Specialty Chemicals
Cyasorb® 531	Cytek
Lowilite® 22	Chemtura Corporation

Physical Properties

Appearance	Yellowish powder					
Melting Point	48-49 °C		Boiling Point >300 °C Decomposes			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH 2	EtOH 2	Acetone 70	CH₂Cl₂ 67	Hexane 25

Application, Regulatory & Environmental Information

Application
 2-Hydroxy-4-n-octyloxybenzophenone is an effective photostabilizer for a variety of plastic systems. It may be used in food packaging materials as an antioxidant and stabilizer and in addition may be used as a stabilizer in petroleum wax. When used in packaging materials, it prevents UV-radiation from reaching the stored product and increases the stability of the container.

Regulatory Information

Approved by the FDA under the 21CFR178.2010 for use in aqueous foods, dairy products (water-in-oil emulsions), bakery products without oil, and dry foods without oil at a maximum concentration of 0.5%.

Environmental Impact

This product is toxic to aquatic organisms and should not be released into the environment. It is not readily biodegradable and has a medium potential to bioaccumulate based on the estimated log Kow value of >6.0.

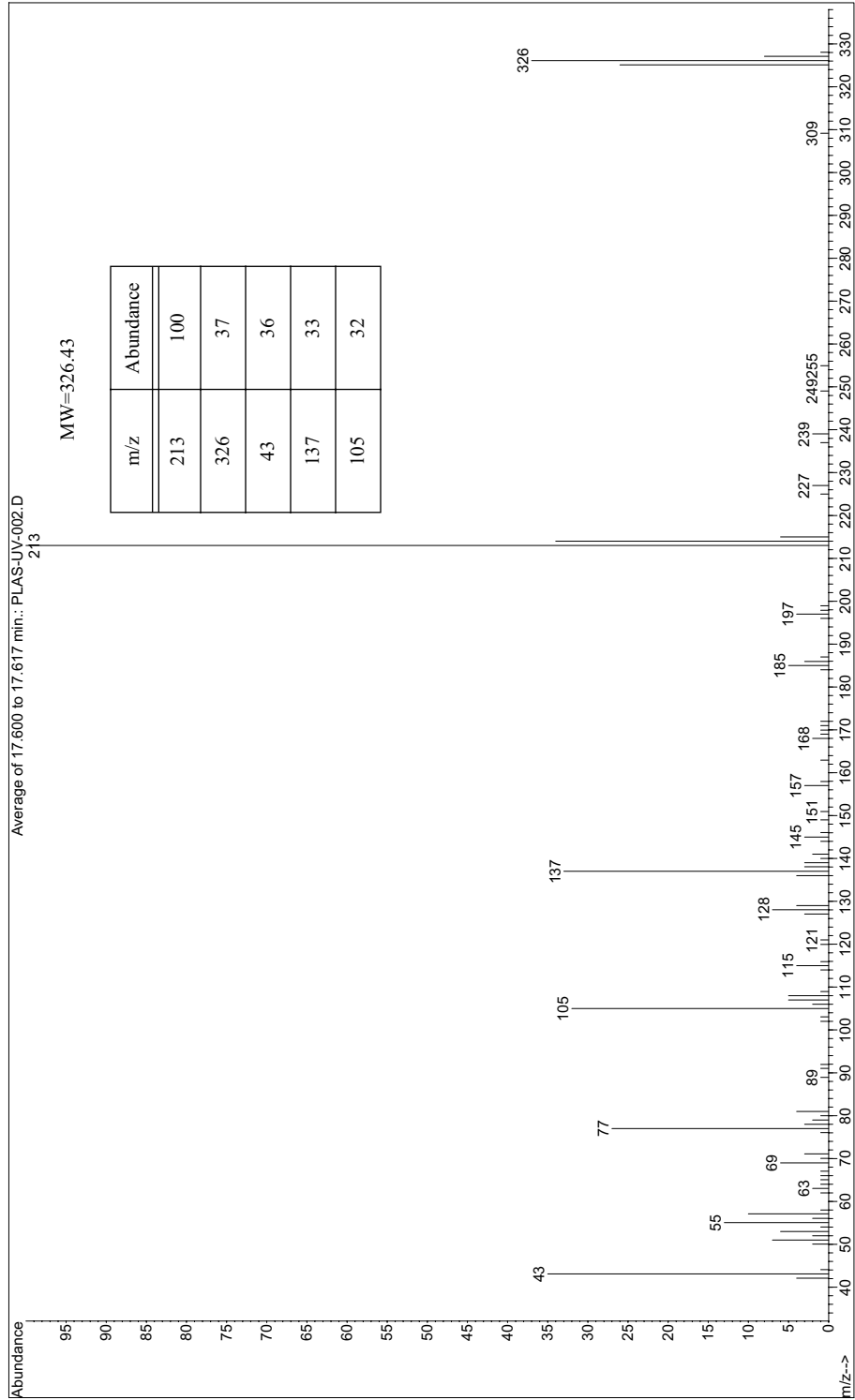
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): >10 g/kg [Rat]; acute dermal (LD50): >10 g/kg [Rabbit]. There are no IARC, OSHA, NTP, or ACGIH exposure guidelines available for this product.

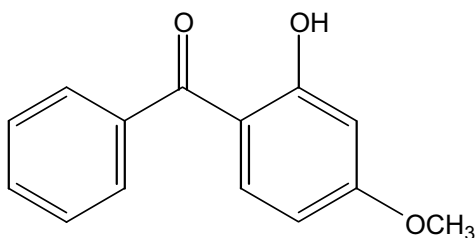
Mass Spectrum for Uvinul® 3008 - PLAS-UV-002



For Chromatogram See Appendix A - PLAS-UV-002 - page 455

Uvinul® 3040

BASF Corporation

**CAS Number** 131-57-7**RTECS Number** DJ1575000**Abbreviation** Not Identified**Formula** C₁₄H₁₂O₃**Molecular Weight** 228.26**Chemical Name**

2-hydroxy-4-methoxybenzophenone

Synonyms

benzophenone compound; oxybenzone; (2-hydroxy-4-methoxyphenyl)phenylmethanone

Brand Names & Manufacturers

Lowilite® 20

Chemtura Corporation

Physical Properties**Appearance** Pale-yellow powder**Melting Point** 62 °C**Boiling Point** 150-160 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	5	5	50	20	U

Application Application, Regulatory & Environmental Information

Uvinul® 3040 is readily compatible with many plastics. It is a particularly effective UV absorber in PVC, acrylic resins, alkyd resins, cellulose nitrate, phenolic resins, and oil colors.

Regulatory Information

Approved by the FDA under 21CFRPart 177 (Indirect Food Additives: Polymers) Subpart B (Substances for Use as Basic Components of Single and Repeated Use Food Contact Surfaces), and Section 177.1010 (Acrylic and modified acrylic plastics, semi-rigid and rigid).

Environmental Impact

Readily biodegradable, but may be inherently toxic to aquatic organisms.

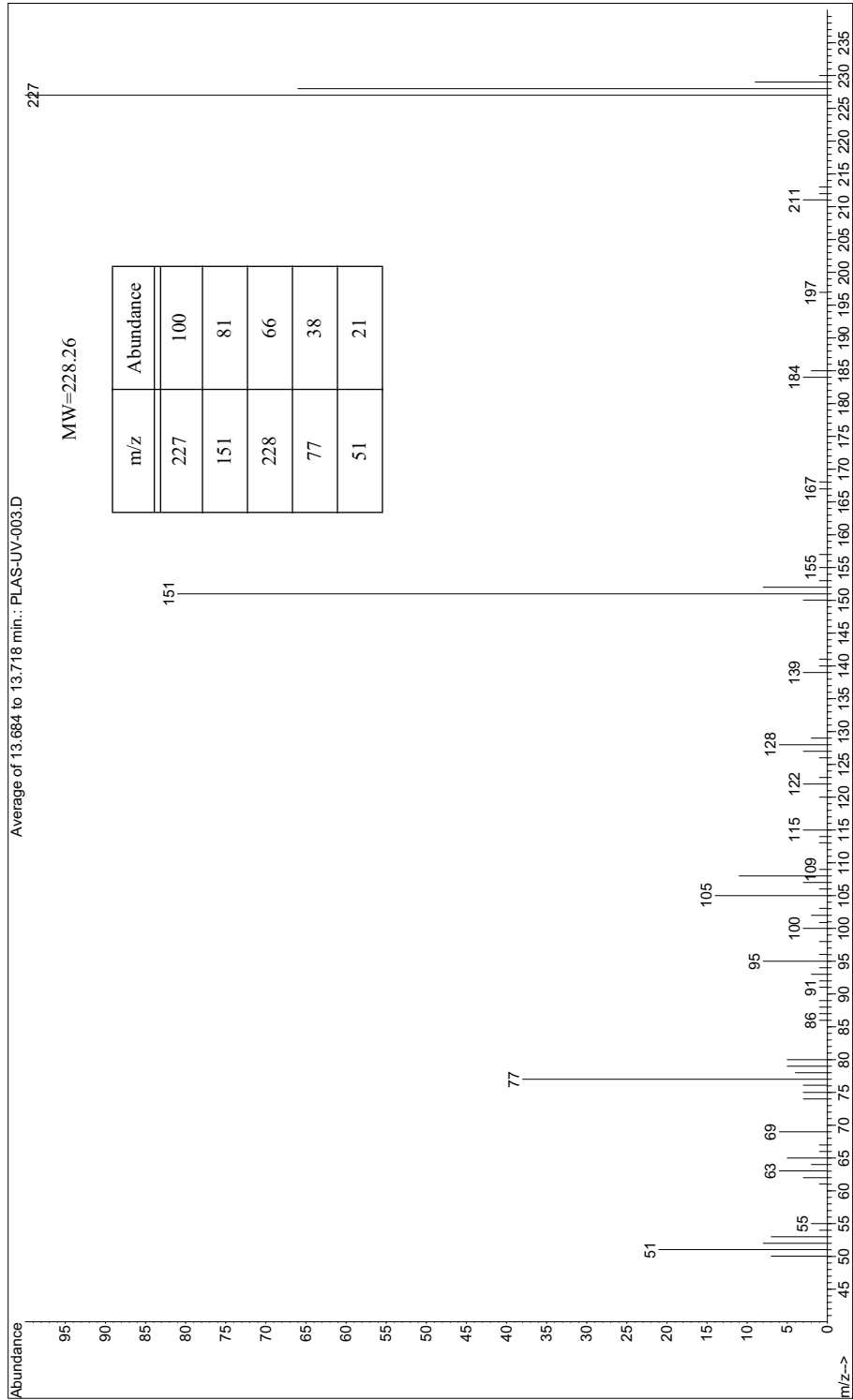
Point of Release

May be absorbed through the skin from cosmetic use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

May cause adverse reproductive effects and may affect genetic material (mutagenic). Lowest Published Toxic Dermal Dose (TDLo): 6500 mg/kg/13W-I [Rat].

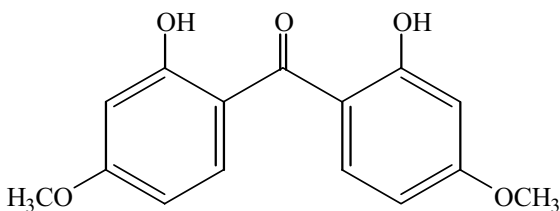
Mass Spectrum for Uvinul® 3040 - PLAS-UV-003



For Chromatogram See Appendix A - PLAS-UV-003 - page 456

Uvinul® 3049

BASF Corporation



CAS Number 131-54-4
RTECS Number DJ0900000
Abbreviation Not Identified

Formula C₁₅H₁₄O₅
Molecular Weight 274.29

Chemical Name

2,2-dihydroxy-4,4-dimethoxybenzophenone

Synonyms

benzophenone compound; bis(2-hydroxy-4-methoxyphenyl)methanone; benzophenone-6

Brand Names & Manufacturers

Helisorb® 11	Norquay
Maxgard® 300	Lycus Ltd.
Unisorb® BP6	UniProma

Physical Properties

Appearance	Pale yellow powder					
Melting Point	131-136 °C		Boiling Point	Decomposes		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH <1	EtOH <1	Acetone U	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application Primarily used as a UV absorber for polyester film. Can also be used in carbonate lenses, SBR rubbers, polyurethane, PET/PETG, PVC, acrylic resins, alkyd resins, epoxy resins, cellulose nitrate, and phenolic resins.

Regulatory Information

This product has FDA approval for food contact applications.

Environmental Impact

This chemical is not considered to be a persistent toxin and has a low potential to bioaccumulate. It is, however, considered to be inherently toxic to aquatic organisms.

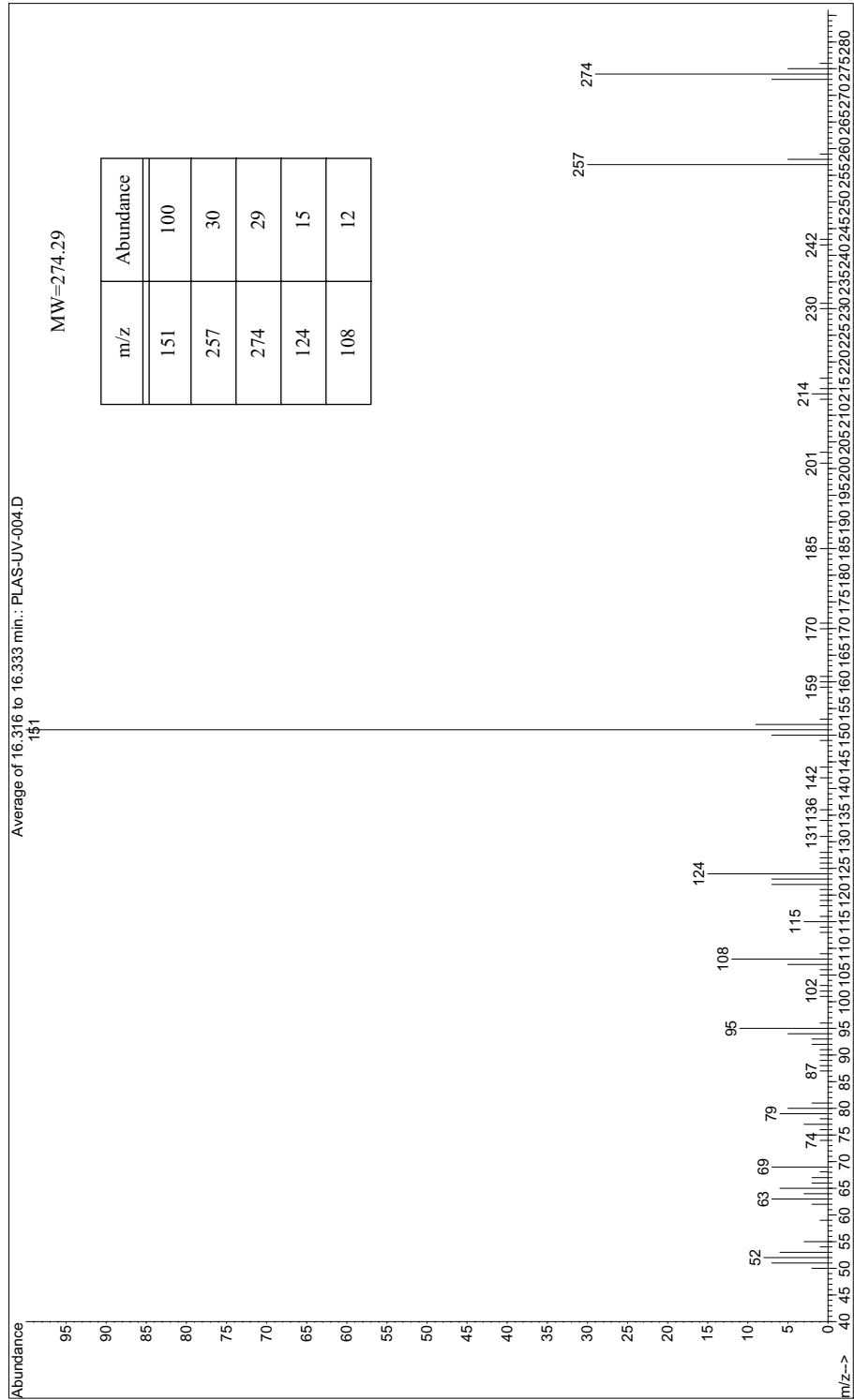
Point of Release

May be absorbed through the skin from cosmetic use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

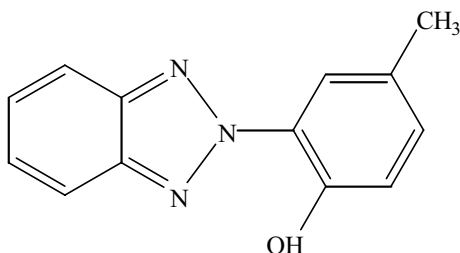
Toxicological Data

Classified as an endocrine disruptor and may cause adverse health effects in humans.

Mass Spectrum for Uvinul® 3049 - PLAS-UV-004



For Chromatogram See Appendix A - PLAS-UV-004 - page 457

Tinuvin® PED

CAS Number 2440-22-4
RTECS Number GO6860000
Abbreviation Not Identified

Formula C₁₃H₁₁N₃O
Molecular Weight 225.27

Chemical Name

2-benzotriazol-2-yl-4-methyl-phenol

Synonyms

2-(2-hydroxy-5-methylphenyl)benzotriazole; 2-(2'-hydroxy-5'-methylphenyl)benzotriazole; drometrizole

Brand Names & Manufacturers

Tinuvin PED

Physical Properties

Appearance	Yellow crystalline powder					
Melting Point	128-133 °C			Boiling Point	225 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH 0.2	EtOH 10	Acetone 3	CH₂Cl₂ 16	Hexane 0.8

Application**Application, Regulatory & Environmental Information**

UV stabilizer particularly effective in styrenic polymers, PVC, unsaturated polyesters, polyurethanes, acrylic polymers, and polycarbonates.

Regulatory Information

Tinuvin® PED has FDA approval for use in a wide variety of food contact applications.

Environmental Impact

This material is not readily biodegradable. If released into the environment, it is expected to partition mainly into the soil due to its insolubility in water. It is considered to be non-toxic to aquatic organisms and its potential to bioaccumulate is low.

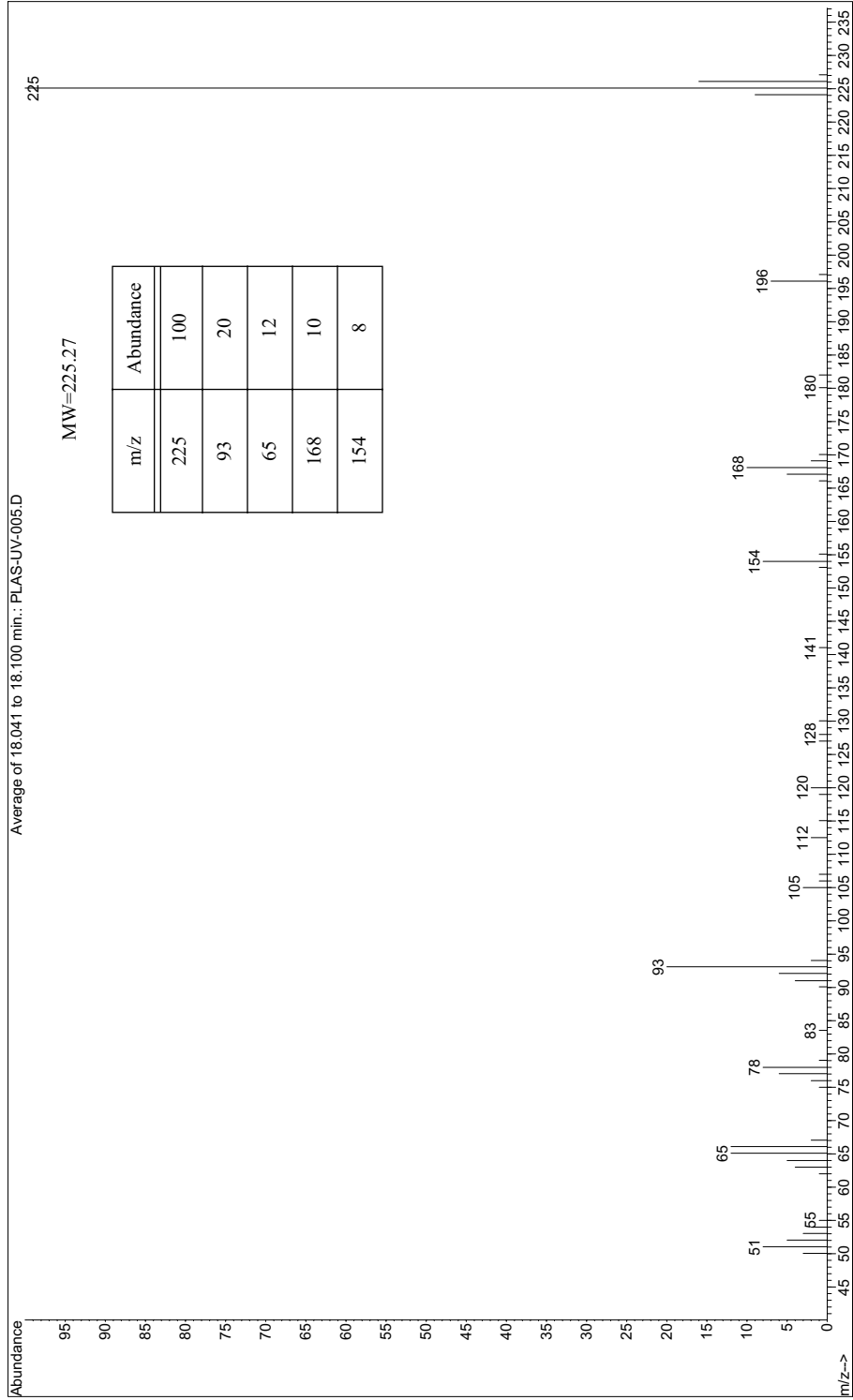
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Primary Irritant. Acute oral toxicity (LD50): 6500 mg/kg [Mouse]. Lowest Published Toxic Oral Dose (TDLo): 270 gm/kg/90D-C [Rat]. Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectrum for Tinuvin® PED - PLAS-UV-005



For Chromatogram See Appendix A - PLAS-UV-005 - page 458

Antioxidants

Exposure of polymers to heat, light, or atmospheric oxygen can result in significant degradation of the polymer properties during processing, storage, and application. In hydrocarbon polymers, the presence of tertiary hydrogen atoms makes the polymer prone to free radical formation, ultimately resulting in chain scission or crosslinking that degrades performance. Antioxidants are used to terminate these chain reactions by removing radical intermediates. Antioxidants are used in most hydrocarbon polymers including polyethylene, polypropylene, polystyrene, and ABS.

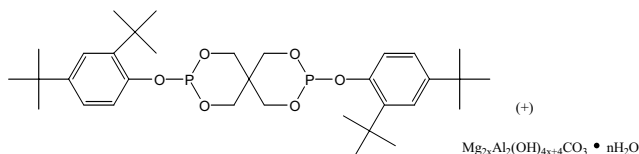
Several factors are typically considered when selecting an antioxidant, including required concentration, compatibility with the host polymer, stability, efficiency, toxicity, ease of use, color change, and cost. Organophosphites are one of the most commonly used antioxidants. They are used to protect the color and molecular weight of the polymer during processing and have been shown to decompose peroxides, as well as chelating and reacting with metals. Reaction with transition metals is of particular interest since these can be catalytically reactive and supportive of oxidative degradation. Other antioxidant groups include sterically hindered phenols (i.e., BHT), thioesters, and amines.

In specialized applications, antioxidant selection becomes constrained by other requirements. In sensitive electrical applications, for example, the electrical conductivity characteristics of antioxidants must be considered. Battery seals are an example, where the antioxidant must have low electrical losses to ensure maximum shelf life of the products. In some applications, long-term exposure to high temperature places stringent requirements on an antioxidant. Appliances are an example, where exposure to high temperature and surfactants can be expected. Antioxidants may be blended in a polymer to provide a range of protection unavailable with a single antioxidant. Antioxidants must be selected on the basis that they will not adversely react with other ingredients in a polymer compound.

Analysis of antioxidants is not necessarily a simple matter. For example, descriptive information about a particular polymer may indicate that a specific antioxidant was added. Analytically, this antioxidant may be found in addition to another. Most commercially supplied base polymers include an antioxidant that is necessary to protect the polymer during initial processing operations, such as pelletizing, crumbling, or extrusion into other pre-forms. The number of commercially available antioxidants is very significant and many types are distinguished by minor changes in the structure. Identification of specific antioxidants requires a large reference library that includes complete mass spectra.

Alkanox® P27

Chemtura Corporation

**CAS Number** 26741-53-7**RTECS Number** N/A**Abbreviation** Not Identified**Formula** $\text{C}_{33}\text{H}_{50}\text{O}_6\text{P}_2$ **Molecular Weight** 604**Chemical Name**

bis(2,4-di-tert-butylphenyl)pentaerythritol diphosphate and magnesium aluminum hydroxy carbonate hydrate

Synonyms

23:2 Mixture of Alkanox® P24 (26741-53-7);magnesium aluminum hydroxy carbonate hydrate (11097-59-9)

Brand Names & Manufacturers

Alkanox P27

Chemtura Corporation

Physical Properties**Appearance** White powder or granules**Melting Point** 160-175 °C**Boiling Point**

Not available

Stability Stable under normal conditions of use.**Solubility**
(g/100mL 20 °C)**Water**
<0.01**MeOH**
~2**EtOH**
U**Acetone**
~11**CH₂Cl₂**
~34**Hexane**
~7**Application, Regulatory & Environmental Information****Application**

Data above for CAS, Formula, and Molecular Weight are for the primary organic molecule — Alkanox® P24.

Decomposes peroxides during processing and reduces activity of catalyst residues, which reduces peroxide formation. Suitable for polyolefins as well as other plastics, elastomers, and adhesives.

Regulatory Information

Listed as having broad approval for indirect food contact in many countries including US, Canada, Europe, and Japan.

Environmental Impact

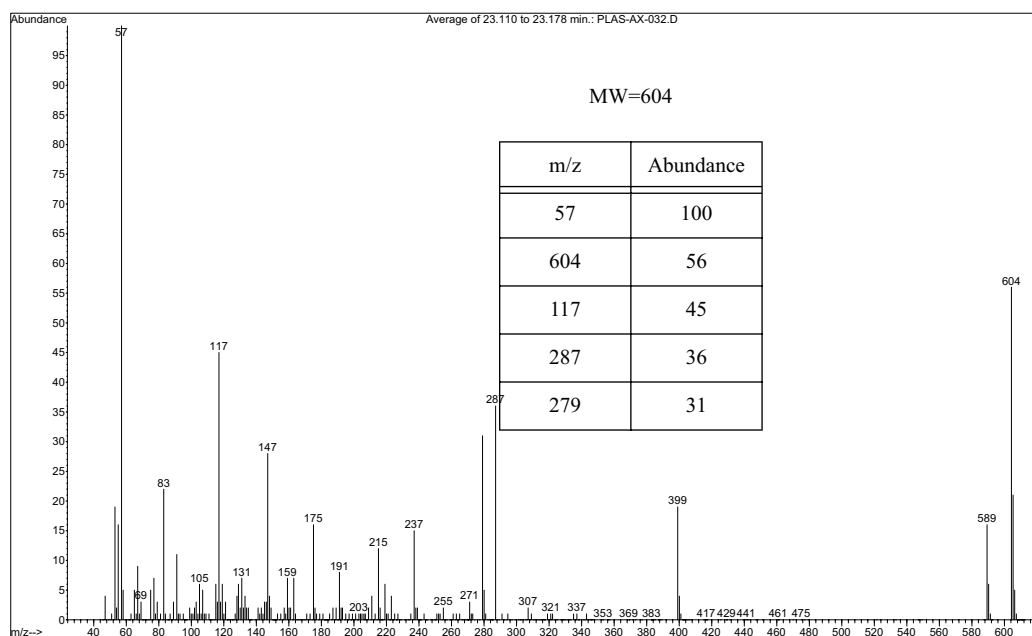
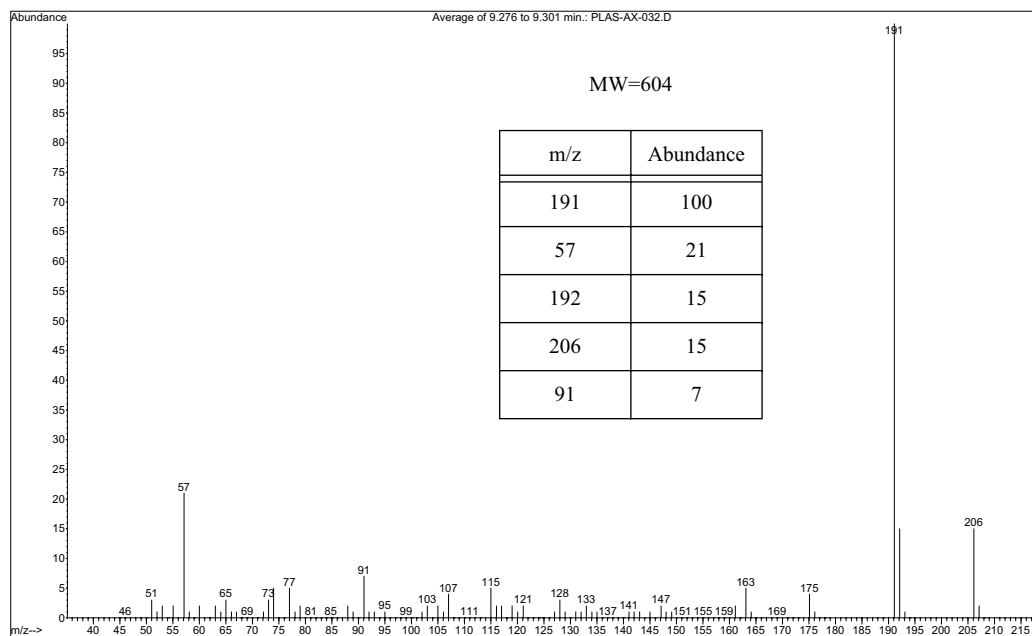
Hydrolysis may produce hindered phenols, which are irritating to the eyes, skin, and mucous tract.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

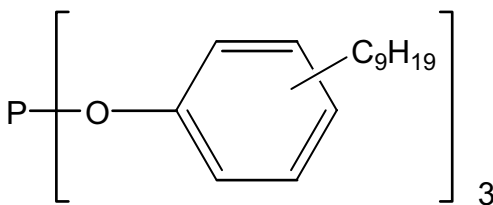
Alkanox® P24: This material has been evaluated as a probable neurotoxin. In a 90-day feeding study with rats dosed at 100, 300, and 1000 ppm levels, no effects were seen with the exception of very slight to slight extramedullary hematopoiesis in liver and spleen of animals fed the highest dose. In a 2 year feeding study in rats at 100 and 500 ppm in the diet, no effects were observed. The material is reportedly not a carcinogen, mutagen, or teratogen.

Mass Spectra for Alkanox[®] P27 - PLAS-AX-032

For Chromatogram See Appendix A - PLAS-AX-032 - page 459

Alkanox® TNPP

Chemtura Corporation

**CAS Number** 26523-78-4**RTECS Number** N/A**Abbreviation** TNPP**Formula** C₄₅H₆₉O₃P**Molecular Weight** 689.00**Chemical Name**

tris(mono-nonylphenyl) phosphite with up to 1% triisopropanol amine

Synonyms

Tris nonylphenyl phosphite; tris(mono-nonylphenyl) phosphite; nonylphenyl phosphite (3:1)

Brand Names & ManufacturersNaugard® P
Mark® 1178Chemtura Corporation
Crompton-Witco**Physical Properties****Appearance** Clear yellow liquid**Melting Point** Not available**Boiling Point**

Decomposes @185 °C

Stability Stable under normal conditions of use.**Solubility**
(g/100mL 20 °C)**Water**
<0.01**MeOH**
<2.3**EtOH**
U**Acetone**
>80**CH₂Cl₂**
U**Hexane**
>80**Application****Application, Regulatory & Environmental Information**

TNPP is used as a phosphite antioxidant and a stabilizer for elastomers such as SBR, NBR, and SIS. Used as a stabilizer and a chelator/complexing agent in PC, PE, PP, PVC, copolymers such as ABS (Acrylonitrile-Styrenic based), SBR, and EVA (Ethylene-vinyl acetate) and in polymer latex and other aqueous systems. TNPP also prevents gel formation during polymerization finishing, storage, and factory processing.

Regulatory Information

FDA approved for a variety of food contact applications.

Environmental Impact

(EC50 48 hr): 0.42 mg/mL [Daphnia magna], (LC50 96 hr) < 10 mg/mL [Zebra fish]. (EBC50): > 100 mg/mL [Green Algae], (LC50): > 100 mg/mL [Aerobic bacteria].

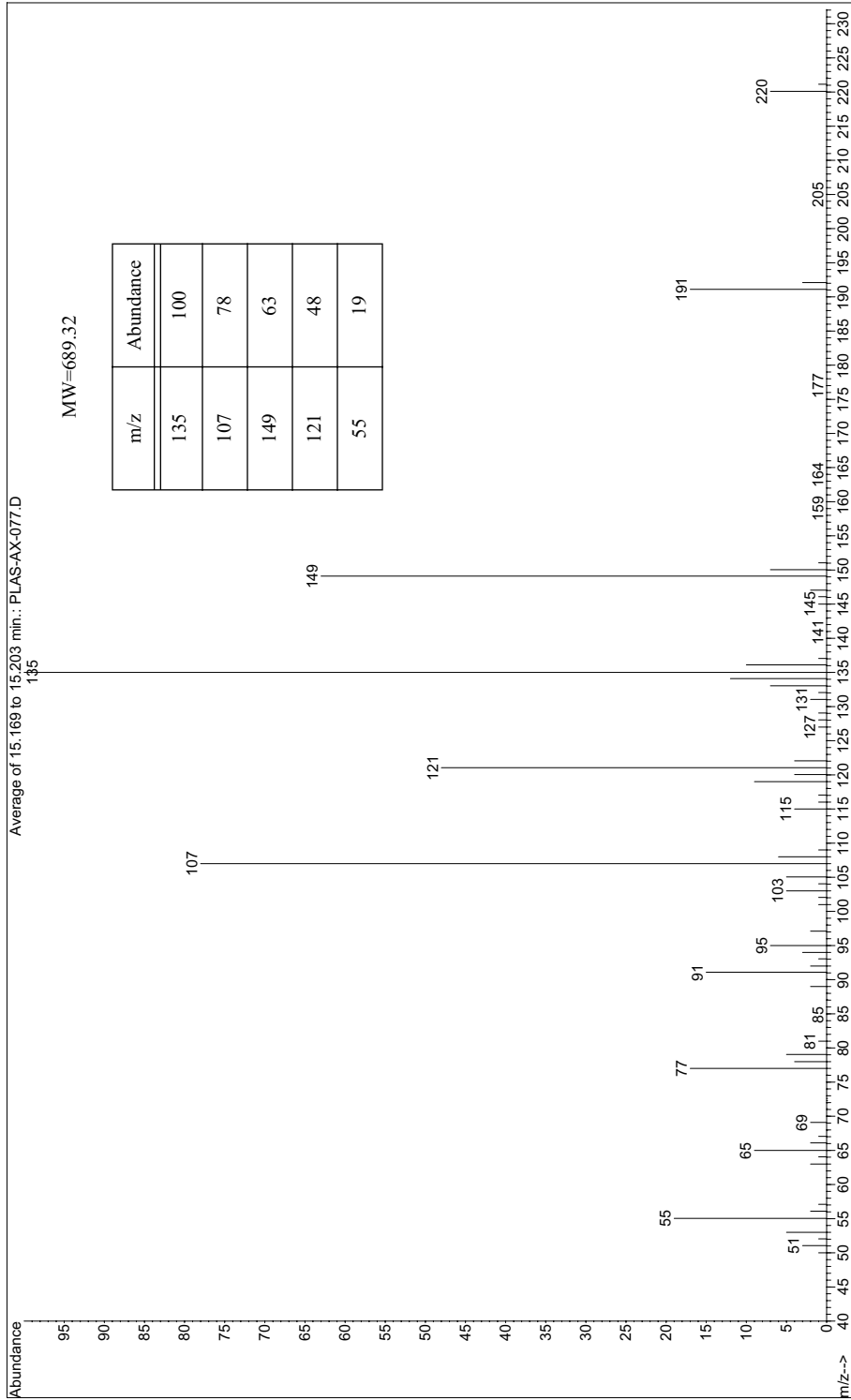
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

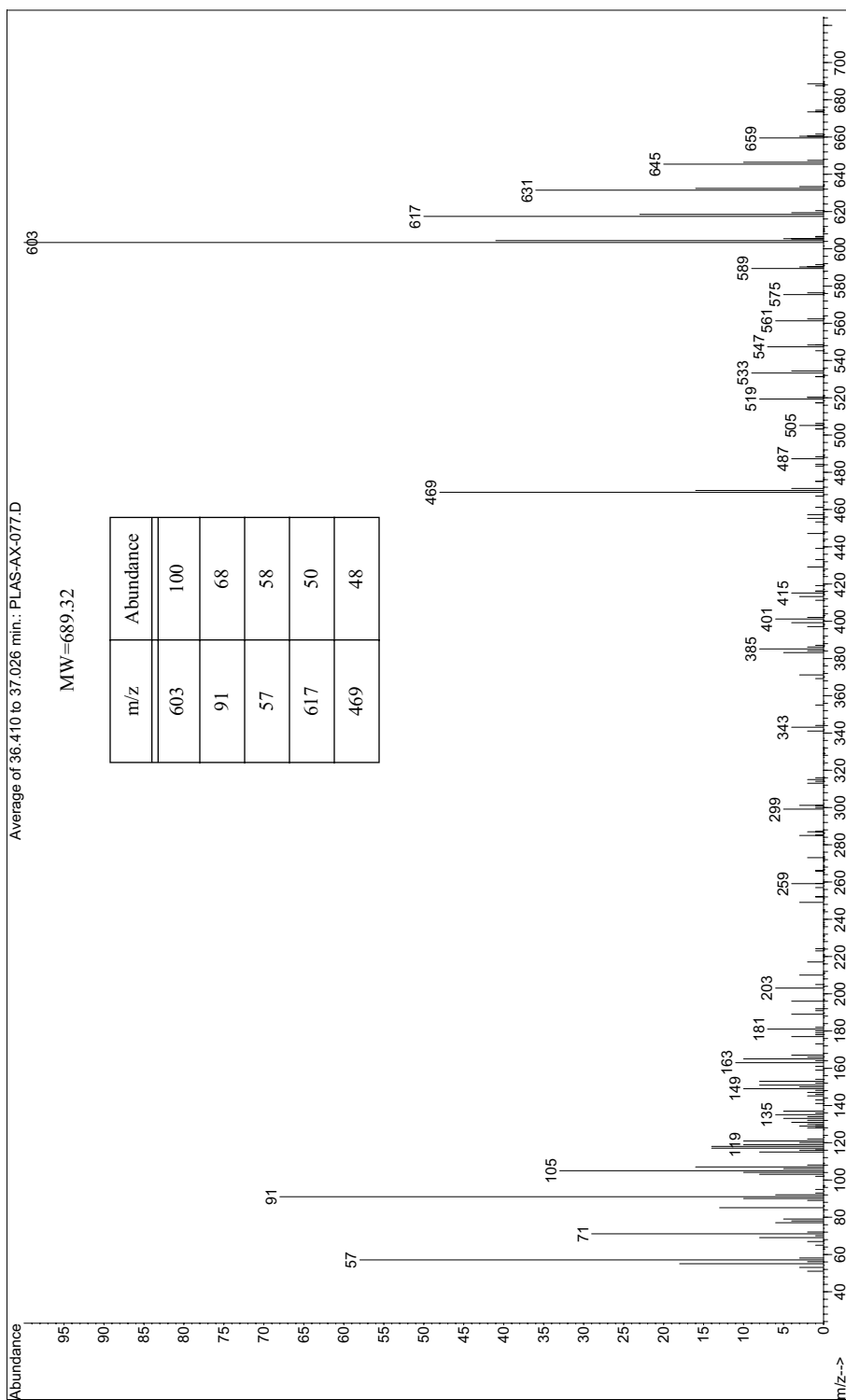
Toxicological Data

May be toxic to kidney based on laboratory animal testing. Irritating to the gastrointestinal system and upper respiratory tract if overexposed. Not reported as carcinogenic.

Mass Spectrum for Alkanox® TNPP - PLAS-AX-077

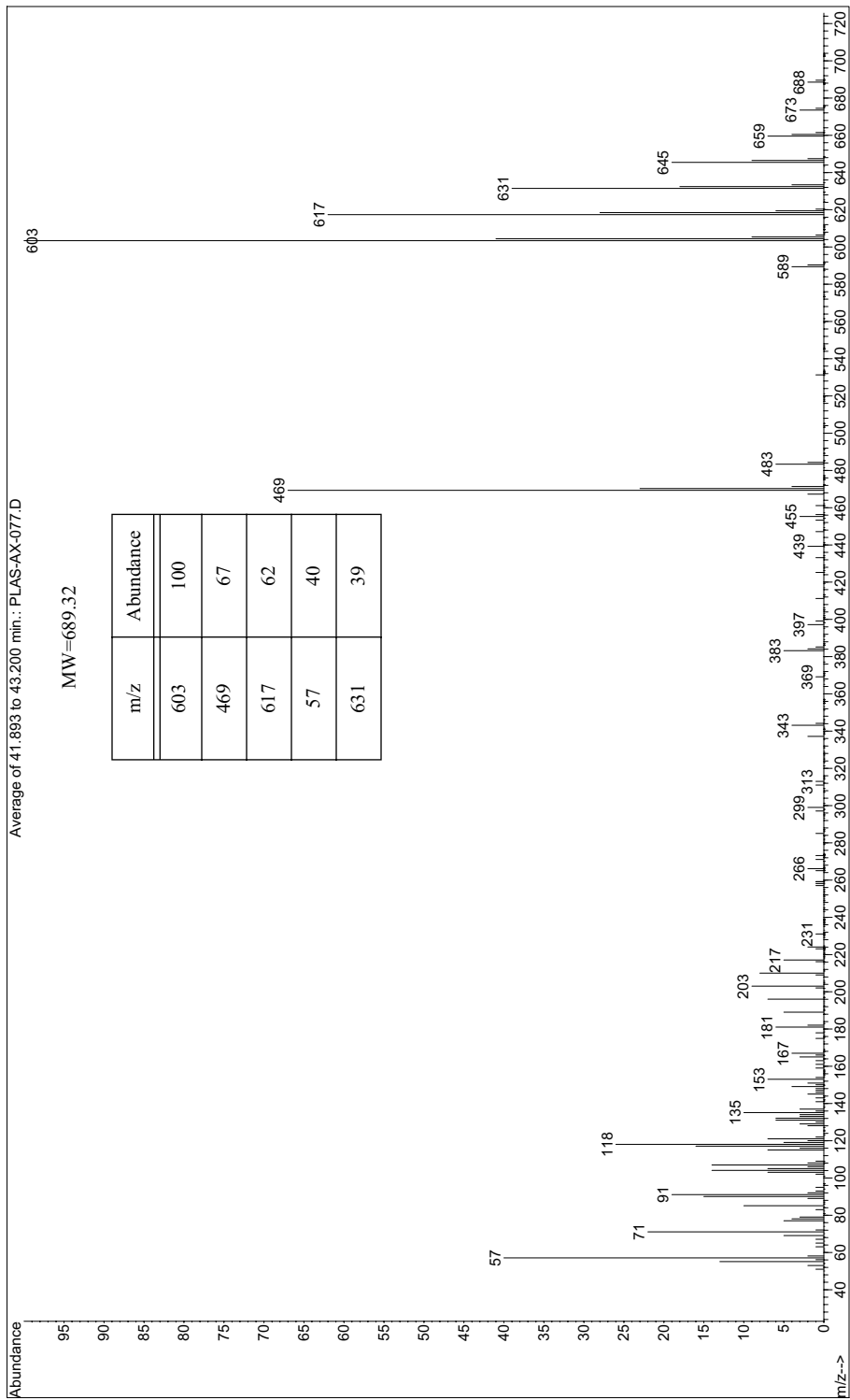


For Chromatogram See Appendix A - PLAS-AX-077 - page 460

Mass Spectrum for Alkanox[®] TNPP - PLAS-AX-077

For Chromatogram See Appendix A - PLAS-AX-077 - page 460

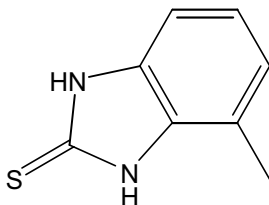
Mass Spectrum for Alkanox® TNPP - PLAS-AX-077



For Chromatogram See Appendix A - PLAS-AX-077 - page 460

Antioxidant 60

Akrochem Corporation

**CAS Number** 53988-10-6**RTECS Number** DE1176050**Abbreviation** MMBI**Formula** C₈H₈N₂S**Molecular Weight** 164.23**Chemical Name**

2H-benzimidazole-2-thione, 1,3-di-hydro-4(or 5)-methyl

Synonyms

1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione; 2-mercaptotoluimidazole; 2-mercapto-4(5)-methyl-benzimidazole

Brand Names & Manufacturers

Tinuvin® 622

Nocrac™ MMB

Vulkanox® MB-2

R.T. Vanderbilt Company, Inc.

Ohuchi Shinko Co., Ltd.

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** White to off-white powder**Melting Point** > 250 °C**Boiling Point**

Decomposes

Stability Stable under ordinary conditions of use.**Solubility**
(g/100mL 20 °C)**Water**
<0.01**MeOH**
10-40**EtOH**
10-40**Acetone**
10-40**CH₂Cl₂**
U**Hexane**
U**Application** **Application, Regulatory & Environmental Information**

MMBI is a rubber antioxidant that, in synergy with amine or phenolic antioxidants, protects against oxygen, heat, and metals (especially in thiuram and dithiocarbamate vulcanizates) at the cost of a retarding effect in the vulcanization process and the reduction of modulus. It also confers steam resistance to rubber compounds and has a brightening effect on transparent materials. It is non-staining/coloring and does not bloom.

Regulatory Information

Not approved by the FDA for use in food contact applications.

Environmental Impact

Possibly hazardous short-term degradation products are not likely. However, long-term degradation products may arise. Expected to readily biodegrade. Fish toxicity: (LC50 96 hr): 22 mg/L [Brachydanio rerio]; (LC100 96 hr): 63 mg/L [Brachydanio rerio].

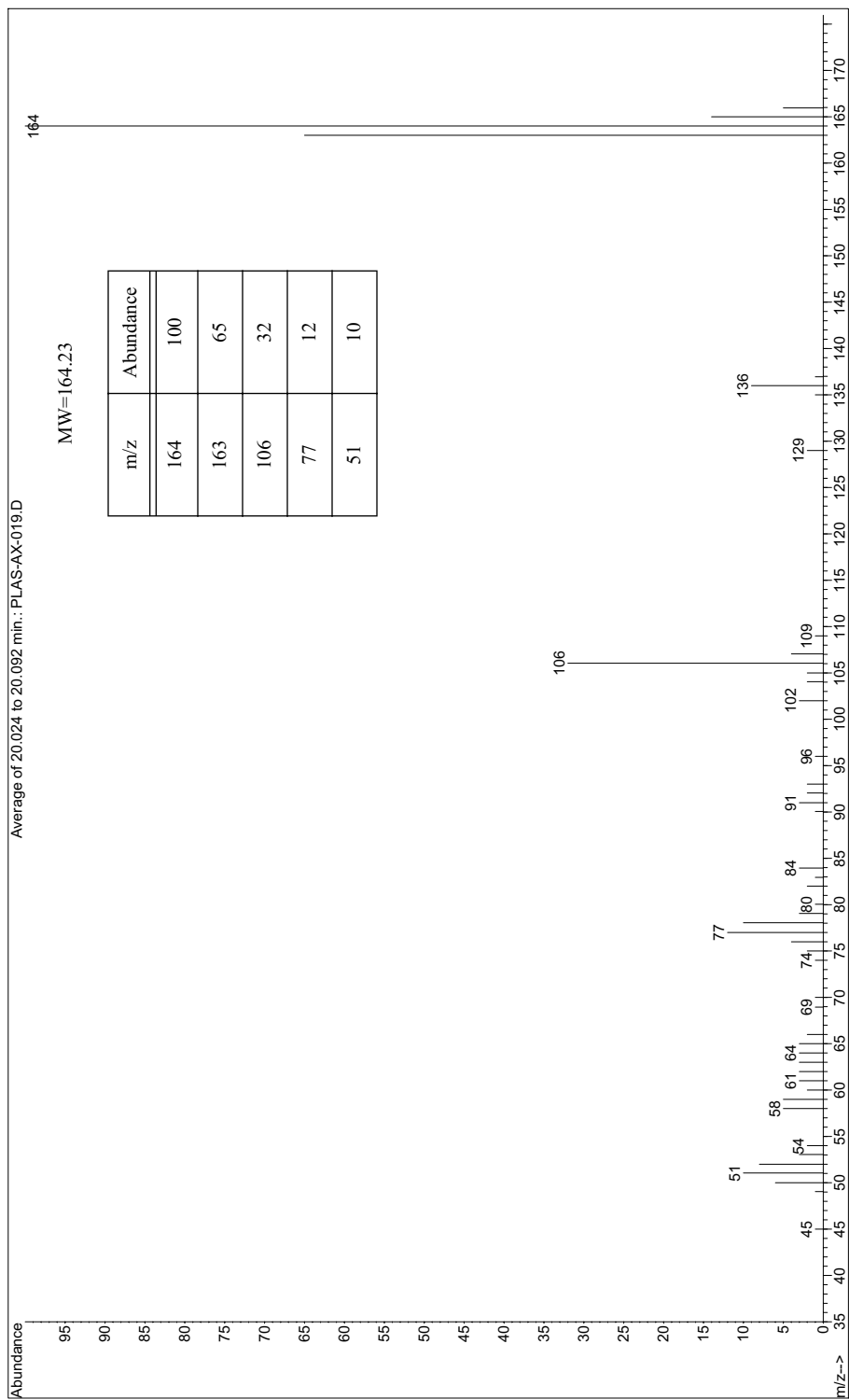
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

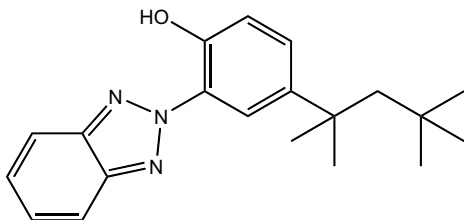
Toxicological Data

MMBI is markedly less toxic than its demethylated compound (MBI or Mercaptobenzoimidazoles). A decrease of thyroid toxicity by methyl substitution of MBI is caused mainly by a decrease in systemic exposure to the compounds and partly by a decrease in inhibition of thyroid hormone synthesis. Oral (LD50): 340 mg/kg [Rat].

Mass Spectrum for Antioxidant 60 - PLAS-AX-019



For Chromatogram See Appendix A - PLAS-AX-019 - page 461

2-(2-Hydroxy-5-*t*-octylphenyl)benzotriazole**CAS Number** 3147-75-9**RTECS Number** MFCD00013338**Abbreviation** Not Identified**Formula** C₂₀H₂₅N₃O**Molecular Weight** 323.43**Chemical Name**

2-(benzotriazol-2-yl)-4-(2,4,4-trimethylpentan-2-yl)phenol

Synonyms

2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol

Brand Names & Manufacturers

BLS® 5411

Mayzo

Tinuvin® 329

Ciba

Physical Properties**Appearance** White crystalline powder**Melting Point** 102-106 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	0.7	U	70.9	U

Application, Regulatory & Environmental Information

Application Provides ultraviolet protection in a wide variety of polymeric systems, particularly in polyesters, polyvinyl chlorides, styrenics, acrylics, polycarbonates, and polyvinyl butyral during outdoor weathering. Typical end use applications include molded items, extruded sheets, glazing materials for window lighting, signs, marine, and auto applications.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

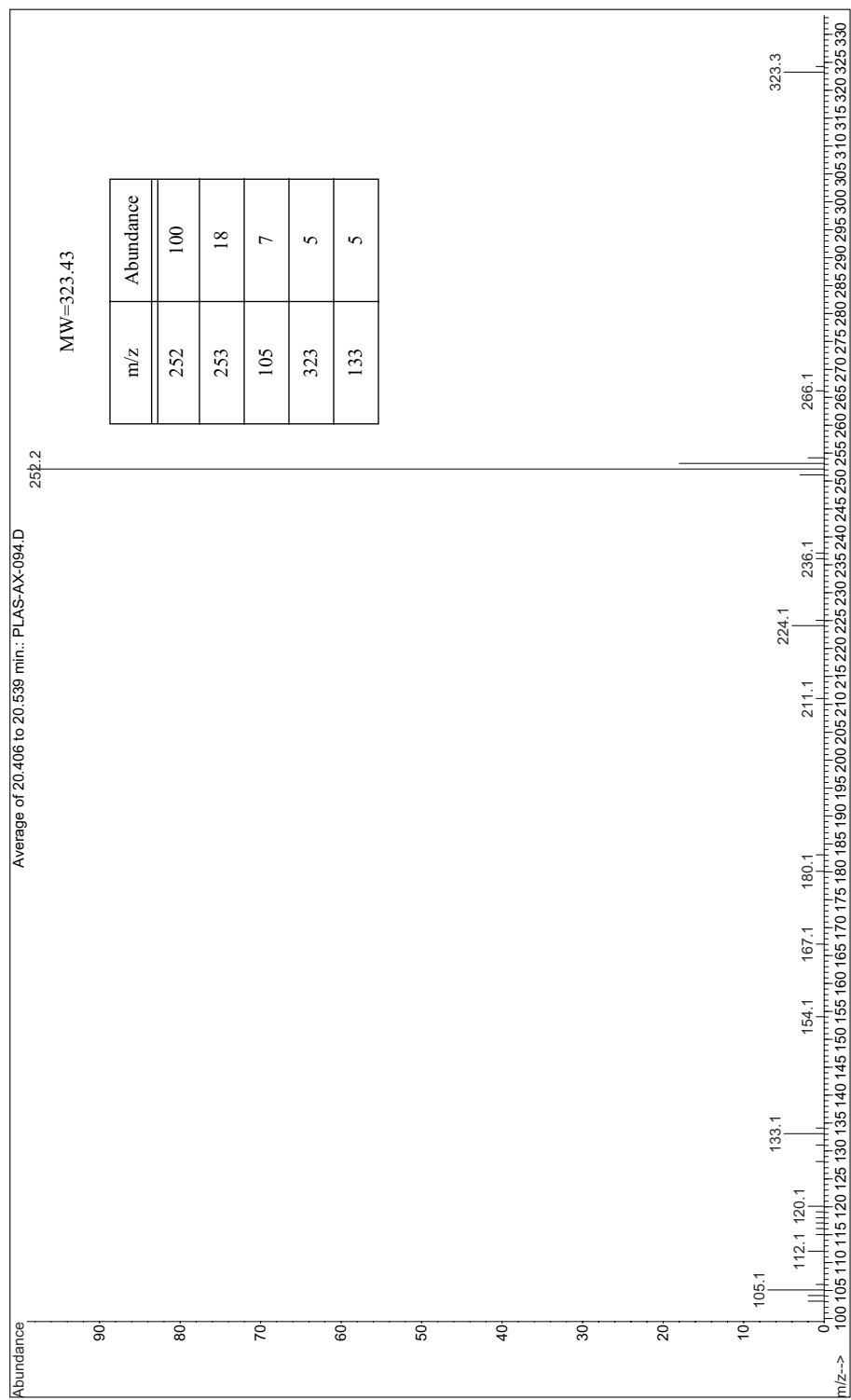
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Toxicological effects are unknown. Repeated and prolonged exposure to this product is not known to aggravate existing medical conditions.

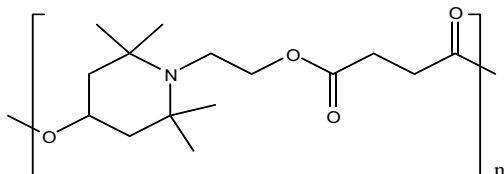
Mass Spectrum for 2-(2-Hydroxy-5-t-octylphenyl)benzotriazole - PLAS-AX-094



For Chromatogram See Appendix A - PLAS-AX-094 - page 462

Mayzo

]



CAS Number 65447-77-0

RTECS Number N/A

Abbreviation Not Identified

Formula (C₁₅H₂₅NO₄)_n

Molecular Weight 283.35

Chemical Name

dimethyl succinate polymer with 4-hydroxy-2,2,6,6-tetramethyl-1-piperidine ethanol

Synonyms

N/A

Brand Names & Manufacturers

Tinuvin® 622

Ciba (BASF)

Physical Properties**Appearance** White to yellow granular powder**Melting Point** 50-70 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.05	0.08	4	>40.0	<0.01

Application, Regulatory & Environmental Information**Application**

Favorable for applications where low volatility and a low melting range are required. It is highly effective in pigmented systems and systems using carbon black. Typical end use applications include adhesives, sealants, elastomers, fibers, and films.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body. Cleared by the FDA for use as an indirect food additive in food packaging and/or other applications.

Environmental Impact

LC50 (catfish, carp, bluegill, and rainbow trout) (96 hour): >100 ppm

LC50 (daphnia magna) acute 24 hour: 25 ppm

Not bioaccumulative or biodegradable.

Point of Release

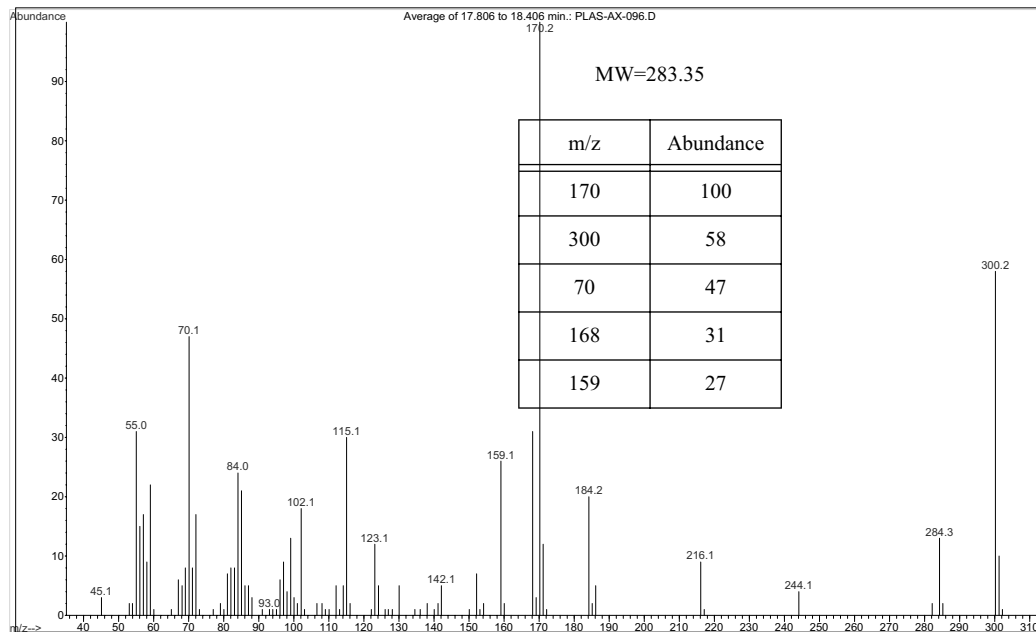
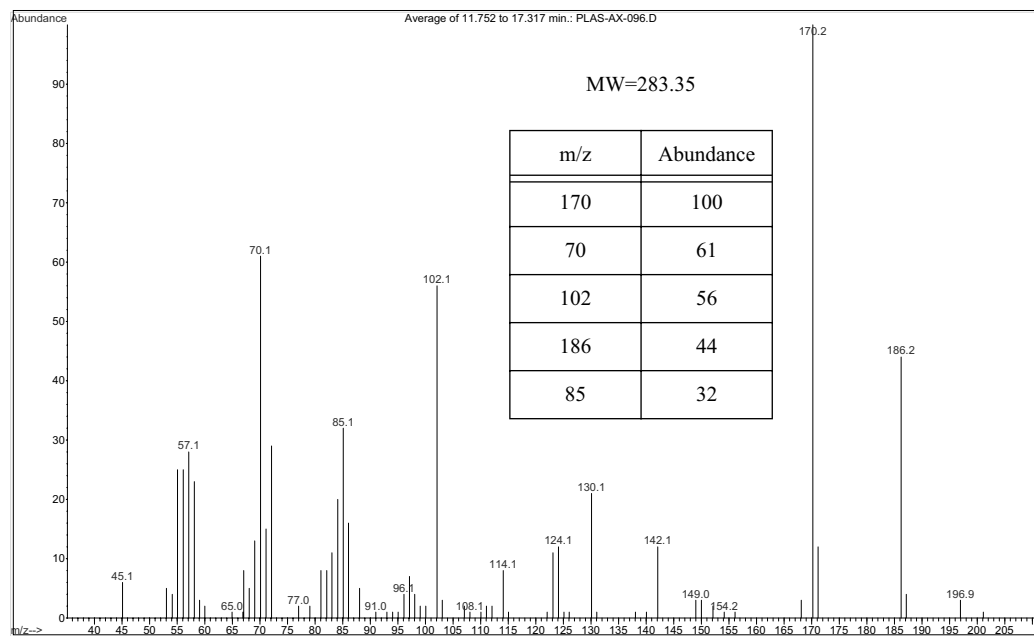
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

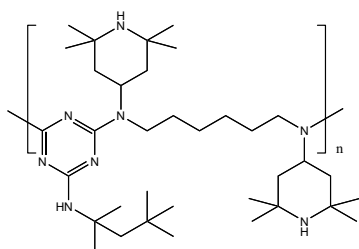
Oral LD50 (rats): >2000 mg/kg

Inhalation LC50 (rats): 1.1 mg/L

Intraperitoneal LD50 (rats): >1000 mg/kg

Mass Spectra for BLS 1622 - PLAS-AX-096N

For Chromatogram See Appendix A - PLAS-AX-096 - page 463

BLS 1944**Mayzo****CAS Number** 70624-18-9**RTECS Number** N/A**Abbreviation** Not Identified**Formula** (C₃₅H₆₆N₈)_n**Molecular Weight** (599.09)_n**Chemical Name**

poly[[6-[(1,1,3,3-tetramethylbutyl)aminol]-s-triazine-2,4-diyl][(2,2,6,6-tetramethyl-4-piperidyl)imino]]hexamethylylene[(2,2,6,6-tetramethyl-4-piperidyl)imino]

Synonyms

hindered amine light stabilizer

Brand Names & Manufacturers

Chimassorb 944

Ciba

Horsorb 944

Sunny Chemical

Physical Properties**Appearance** White to yellow pastille**Melting Point** 100 - 135 °C**Boiling Point**

N/A

Stability Stable under normal conditions of use.**Solubility**
(g/100mL 20 °C)**Water**
<0.01**MeOH**
3**EtOH**
<0.1**Acetone**
>50**CH₂Cl₂**
>50**Hexane**
41**Application****Application, Regulatory & Environmental Information**

Polymeric hindered amine light stabilizer is excellent for protection against ultraviolet degradation. Applications include polyolefins (polypropylene, polyethylene), olefin copolymers such as EVA as well as blends of polypropylene with elastomers. Also effective in polyacetals, polyamides, polyurethanes, flexible and rigid PVC, and PVC blends.

Regulatory Information

FDA cleared for use in food contact applications. It is not intended for use in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Acute aquatic toxicity: 0.35 ppm LC50 in rainbow trout (96 hour); 0.59 ppm LC50 in bluegill (96 hour); 55 mg/L EC50 in Daphnia magna (24 hour); >100 mg/L EC50 in green algae (72 hour)

Not readily biodegradable.

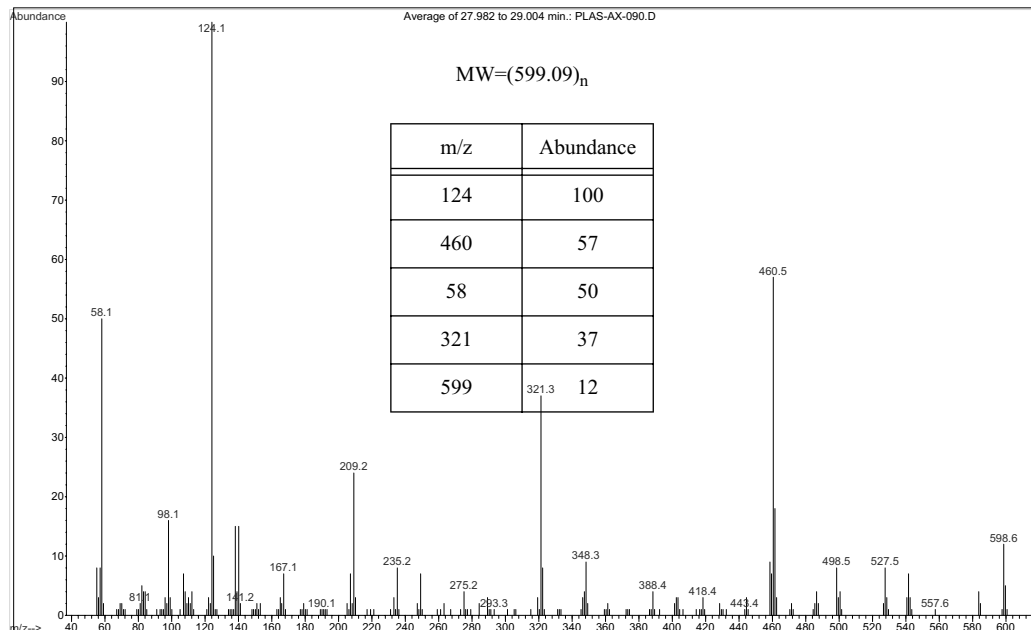
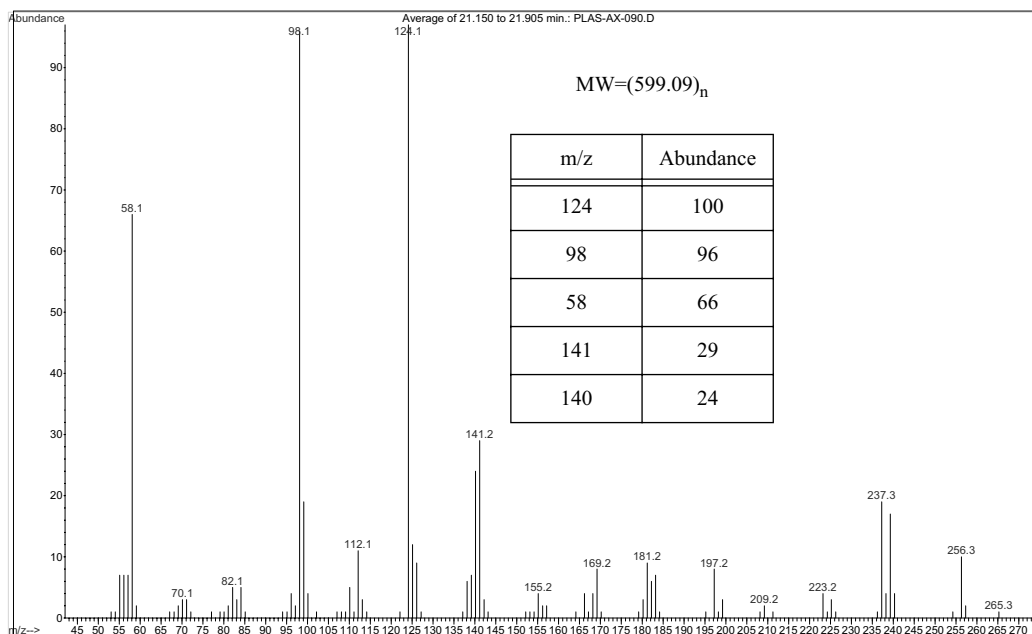
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

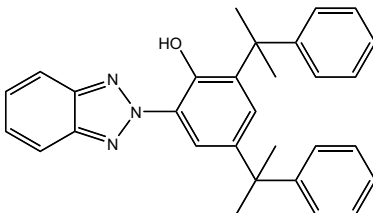
Toxicological Data

> 2000 mg/kg oral-rat LD50

> 3000 mg/kg dermal-rat LD50

Mass Spectra for BLS 1944 - PLAS-AX-090

For Chromatogram See Appendix A - PLAS-AX-090 - page 464

BLS 234**Mayzo****CAS Number** 70321-86-7**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₃₀H₂₉N₃O**Molecular Weight** 447.57**Chemical Name**

2-[2-hydroxy-3,5-di-(1,1-dimethylbenzyl)]-2H-benzotriazole

Synonyms

2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol

Brand Names & Manufacturers

Tinuvin 234

Ciba

Physical Properties**Appearance** Pale yellow powder**Melting Point** 137-141 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	<0.1	0.3	2	34	0.6

Application, Regulatory & Environmental Information**Application**

Especially suited for polycarbonates, polyesters, and other polymers usually processed at high temperatures. In polyolefins, it has a low volatility at high temperatures and high resistance to thermal degradation for polyolefin compounding and molding applications. It is especially suitable for applications of high surface area, such as films and fibers.

Regulatory Information

Not intended for use in products which may come in contact with mucous membranes or abraded skin or be implanted into the body. It does have FDA approval for indirect food contact in most polymers.

Environmental Impact

LC50 (96 hour): >67 ppm [Zebra Fish]

LC50 (24 hour): >91 ppm [Daphnia magna]

EC50 (72 hour): >100 ppm [Green algae]

Not readily biodegradable.

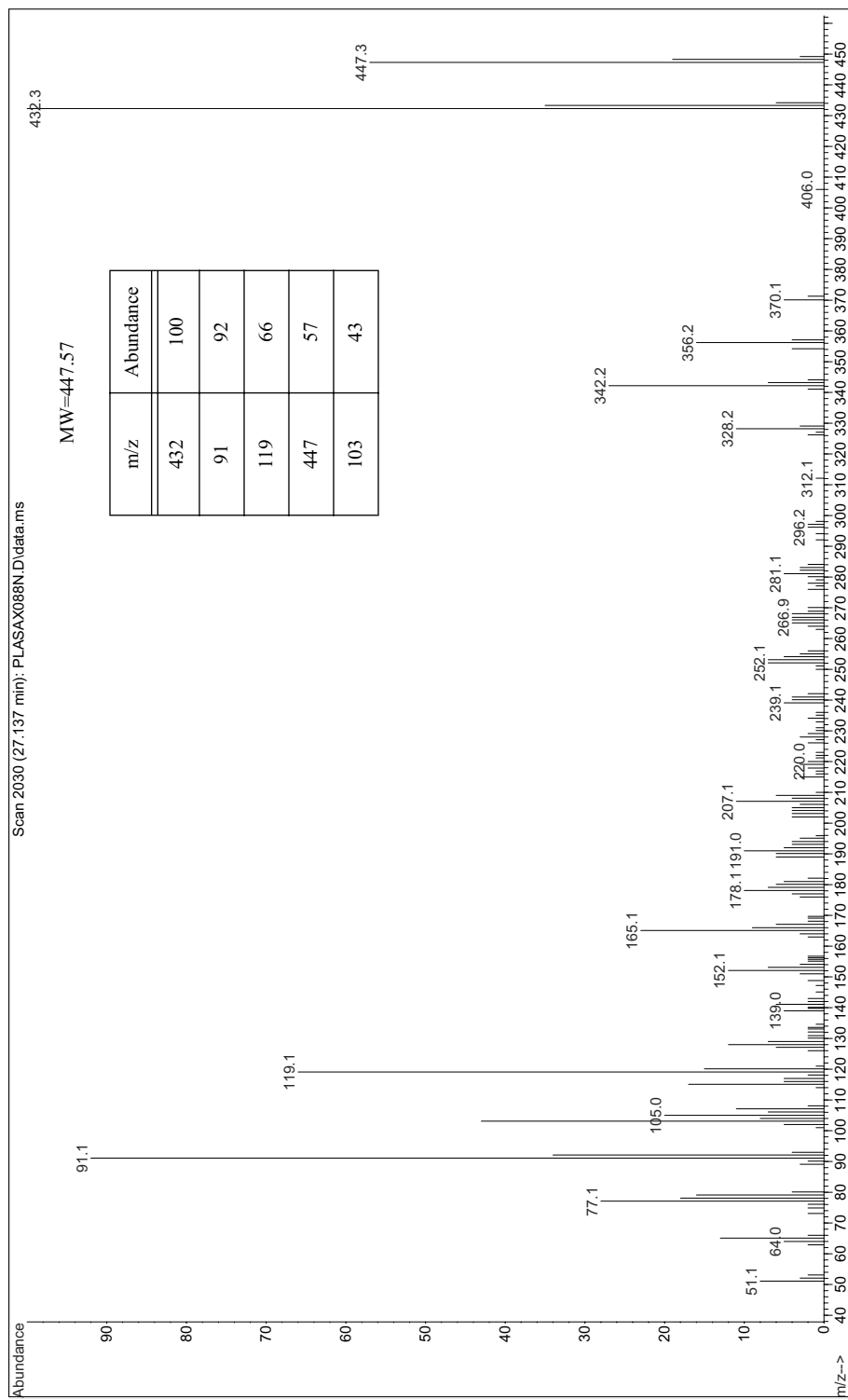
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

NOEL of 50 ppm.

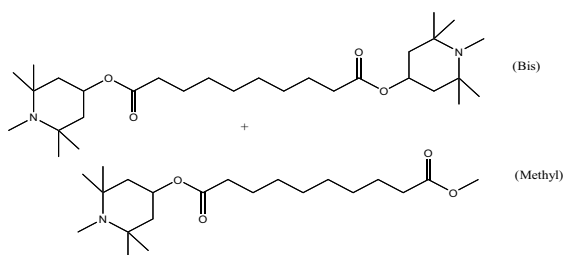
Mass Spectrum for BLS 234 - PLAS-AX-088



For Chromatogram See Appendix A - PLAS-AX-088 - page 465

BLS 292

Mayzo

**CAS Number** 41556-26-7**RTECS Number** N/A**Abbreviation** Not Identified**Formula** $C_{30}H_{56}N_2O_4$ **Molecular Weight** 508.78**Chemical Name**bis (1,2,2,6,6-pentamethyl-4-piperidinyloxy) sebacate • CAS 41556-26-7 • $C_{30}H_{56}N_2O_4$ • 75-85%methyl (1,2,2,6,6-pentamethyl-4-piperidinyloxy) sebacate • CAS 82919-37-7 • $C_{22}H_{39}N_1O_4$ • 15-25%**Synonyms**

N/A

Brand Names & Manufacturers

BLS 292

Mayzo

Physical Properties**Appearance** Light yellow liquid**Melting Point** <20 °C**Boiling Point** >350 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	>50	>50	>50	>50	>50

Application, Regulatory & Environmental Information**Application**

Sterically hindered amine light stabilizer offering excellent protection against ultraviolet degradation. Very effective in coating applications including coil coatings, automotive coatings, paints, inks, and wood stains. Also used in PVB and PVC plastics.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Not readily biodegradable. Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

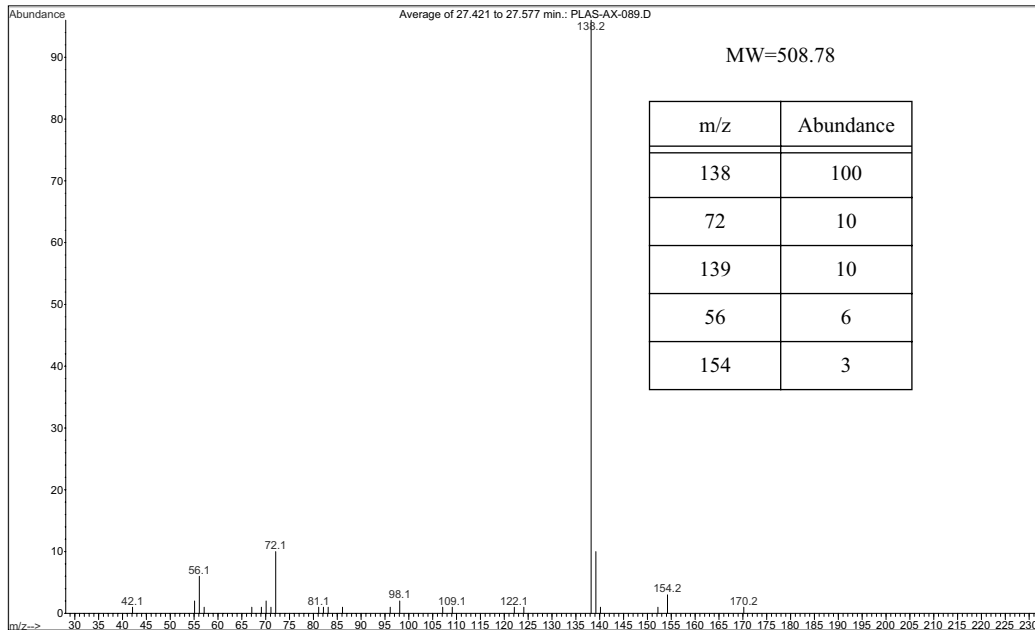
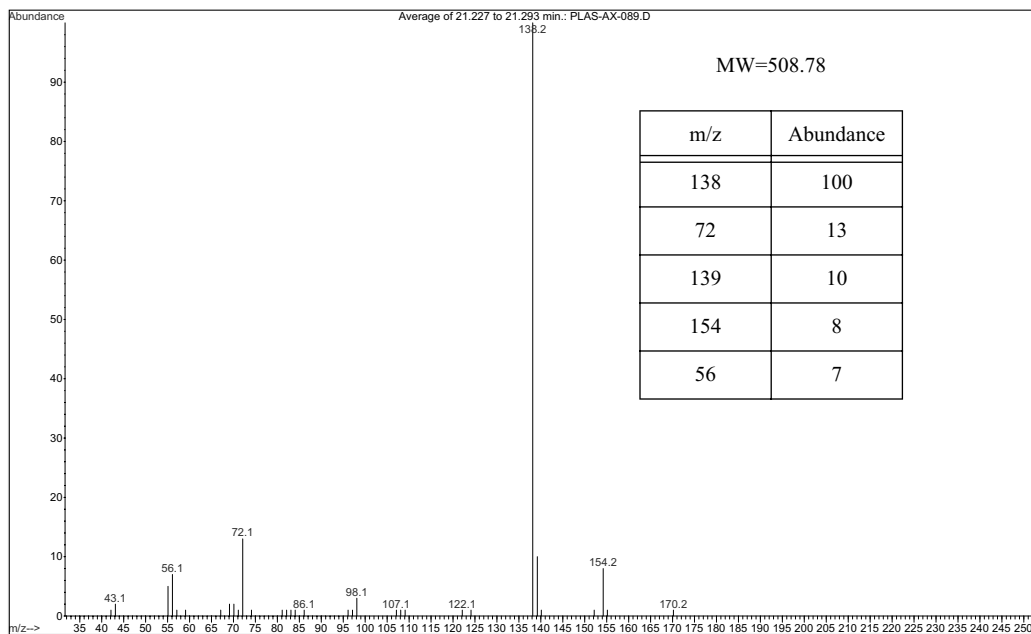
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

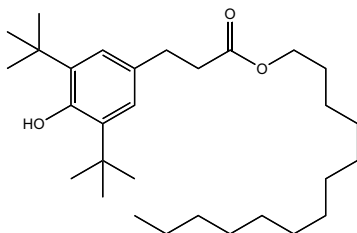
Toxicological Data

LD50 Oral (Rats) > 3g/kg

Strong skin sensitizing potential.

Mass Spectra for BLS 292 - PLAS-AX-089

For Chromatogram See Appendix A - PLAS-AX-089 - page 466

BNX 1077**Mayzo****CAS Number** 847488-62-4**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₃₀H₅₂O₃**Molecular Weight** 460.73**Chemical Name**

benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, isotridecyl ester

Synonyms

N/A

Brand Names & ManufacturersSONGNOX[®] 1077 LQ

RT Vanderbilt

Physical Properties**Appearance** Viscous Liquid**Melting Point** -56 °C**Boiling Point** 230 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	U	U	U

Application **Application, Regulatory & Environmental Information**

Low viscosity liquid antioxidant that can be used as a stabilizer for a variety of polymer applications. It is an excellent antioxidant for PVC polymerization, in polyols for polyurethane foam manufactureres, ABS emulsion polymerization, hot melt adhesives and tackifiers, oils, and resins. The alkyl chain adds compatibility and solubility to various substrates.

Regulatory Information

Not intended for use in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Not readily biodegradable. Contains no hazardous air pollutants or ozone depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

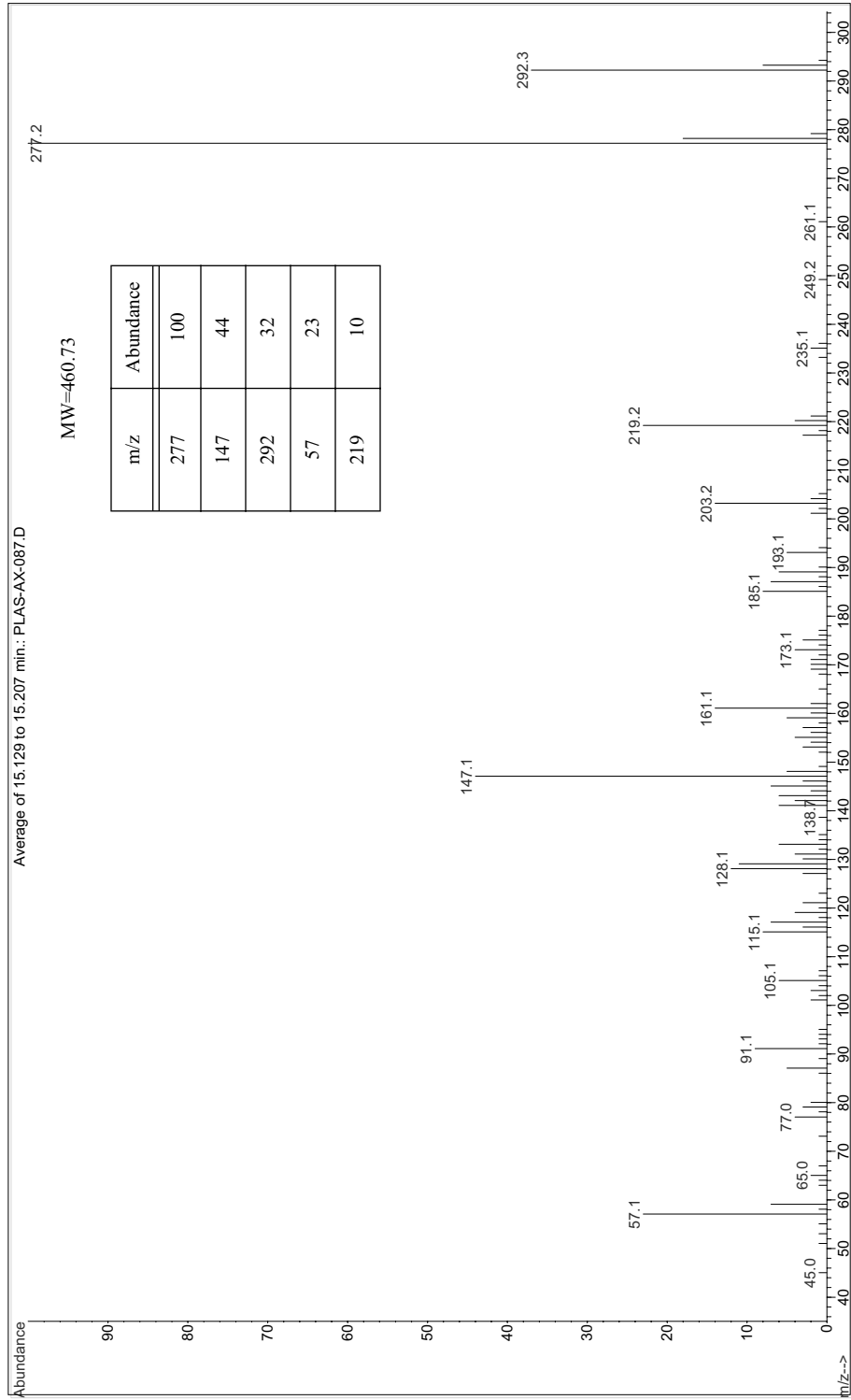
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

LD50 values have not been determined.

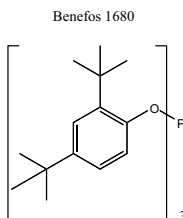
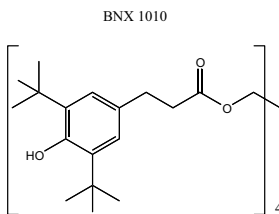
Mass Spectrum for *BNX 1077 - PLAS-AX-087N*



For Chromatogram See Appendix A - PLAS-AX-087 - page 467

BNX 1225 TPR

Mayzo

**CAS Number** See Below**RTECS Number** N/A**Abbreviation** Not Identified**Formula** N/A**Molecular Weight** N/A**Chemical Name**BNS 1010 - tetrakis[methylene-3(3',5-di-tert-butyl-4-hydroxyphenyl)propionate] methane • CAS 6683-19-8 • C₇₃H₁₀₀O₁₂Benefos 1680 - tris(2,4-di-tert-butylphenyl) phosphite • CAS 31570-04-4 • C₄₂H₆₃O₃P**Synonyms**Blend of BNX[®] 1010, Benefos[®] 1680 and SIS Block Copolymer (Proprietary formula)**Brand Names & Manufacturers**Quintac[®] 3620

Zeon Chemicals

Physical Properties**Appearance** Pellets**Melting Point** N/A**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Used in the manufacture of hot-melt pressure sensitive adhesives using single or twin-screw extruders. Can also be used with sigma mixers to achieve a more uniform dispersion of antioxidants.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body. All individual components are approved for food contact applications.

Environmental Impact

Not readily biodegradable.

LC50 (96 hour): >4.05 ppm [Zebra Fish]

LC50 (24 hour): >86 ppm [Daphnia magna]

Point of Release

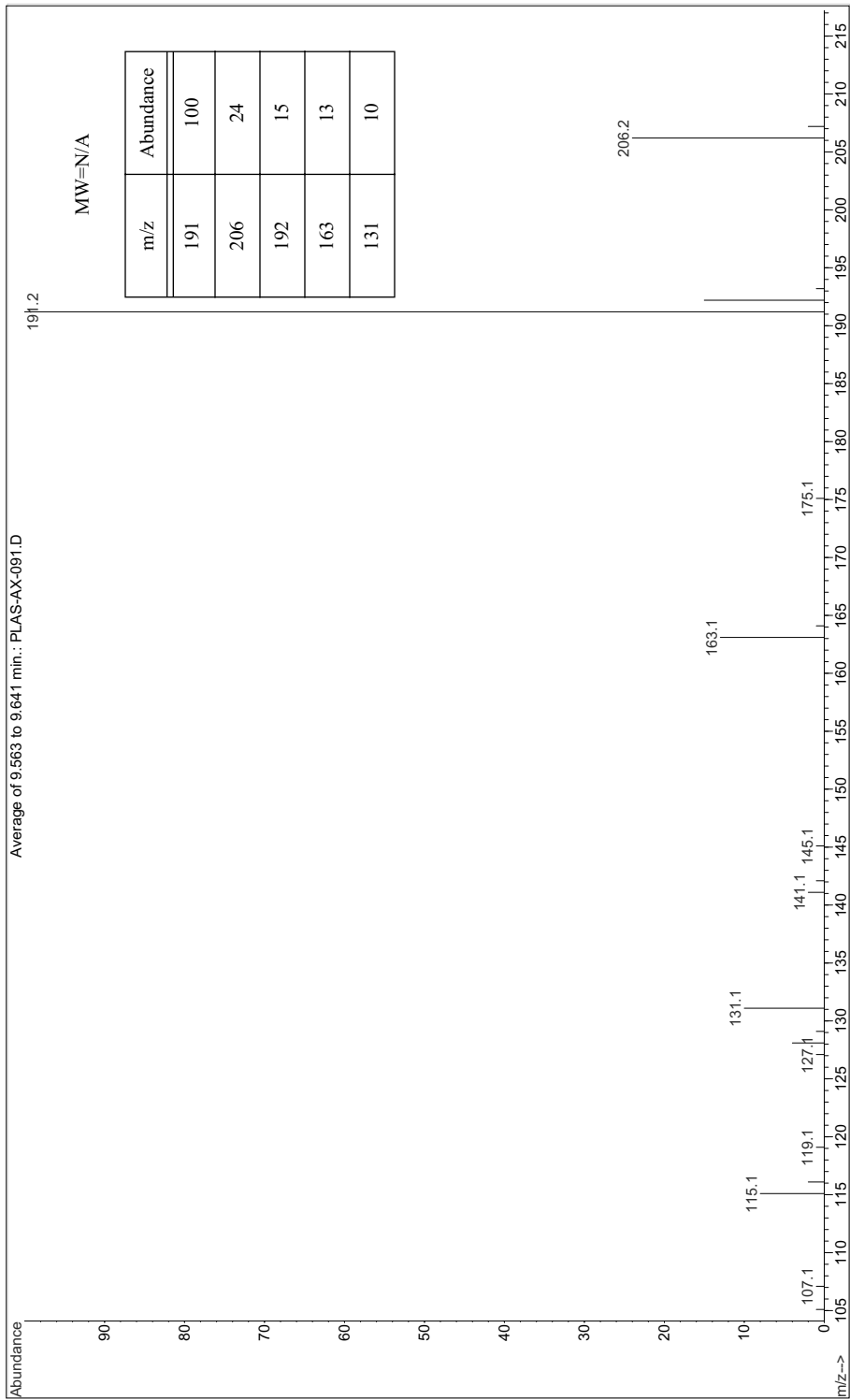
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): > 5,000 mg/kg [Rat]

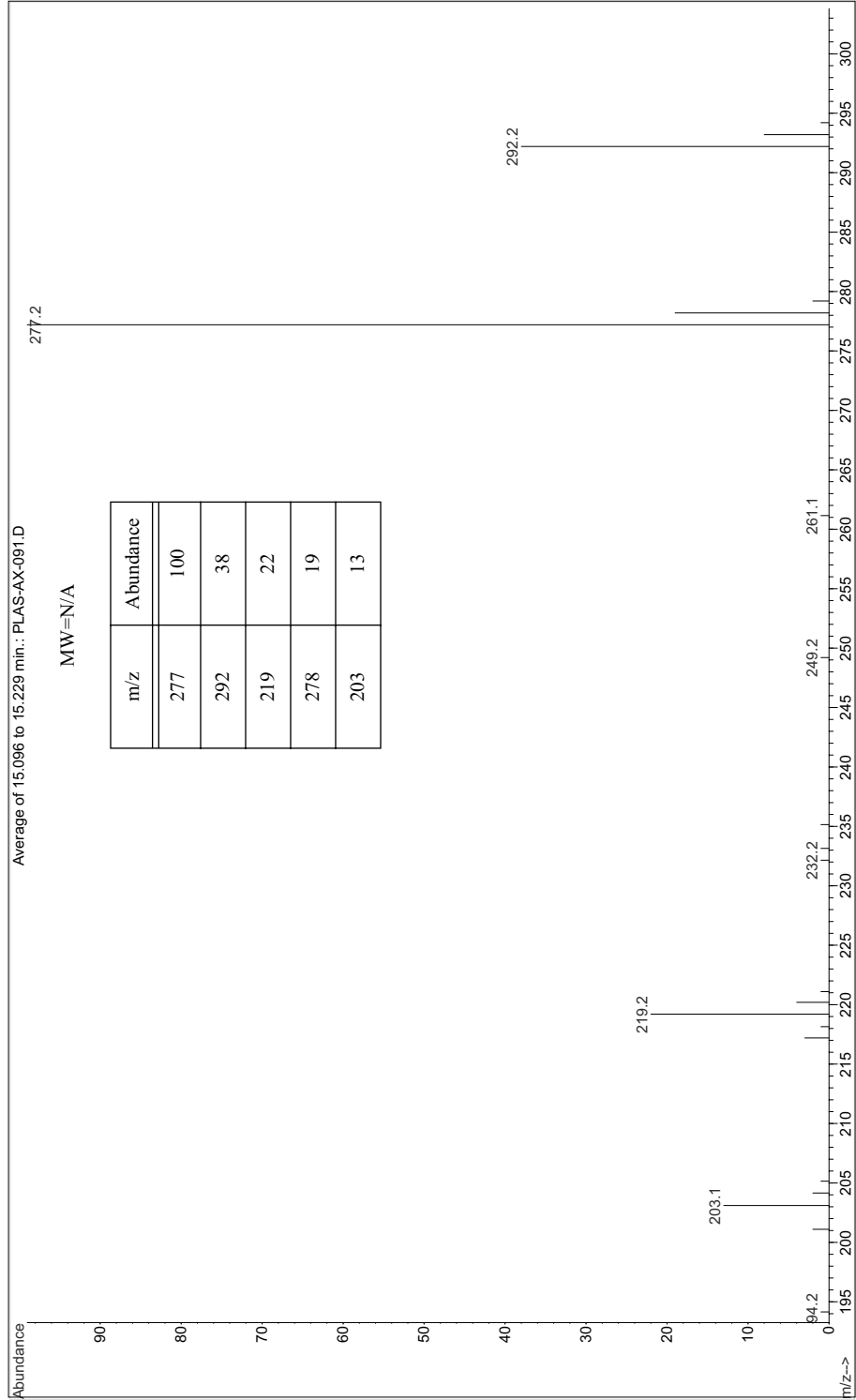
Acute dermal (LD50): > 2,000 mg/kg [Rat]

Mass Spectrum for *BNX 1225 TPR - PLAS-AX-091*



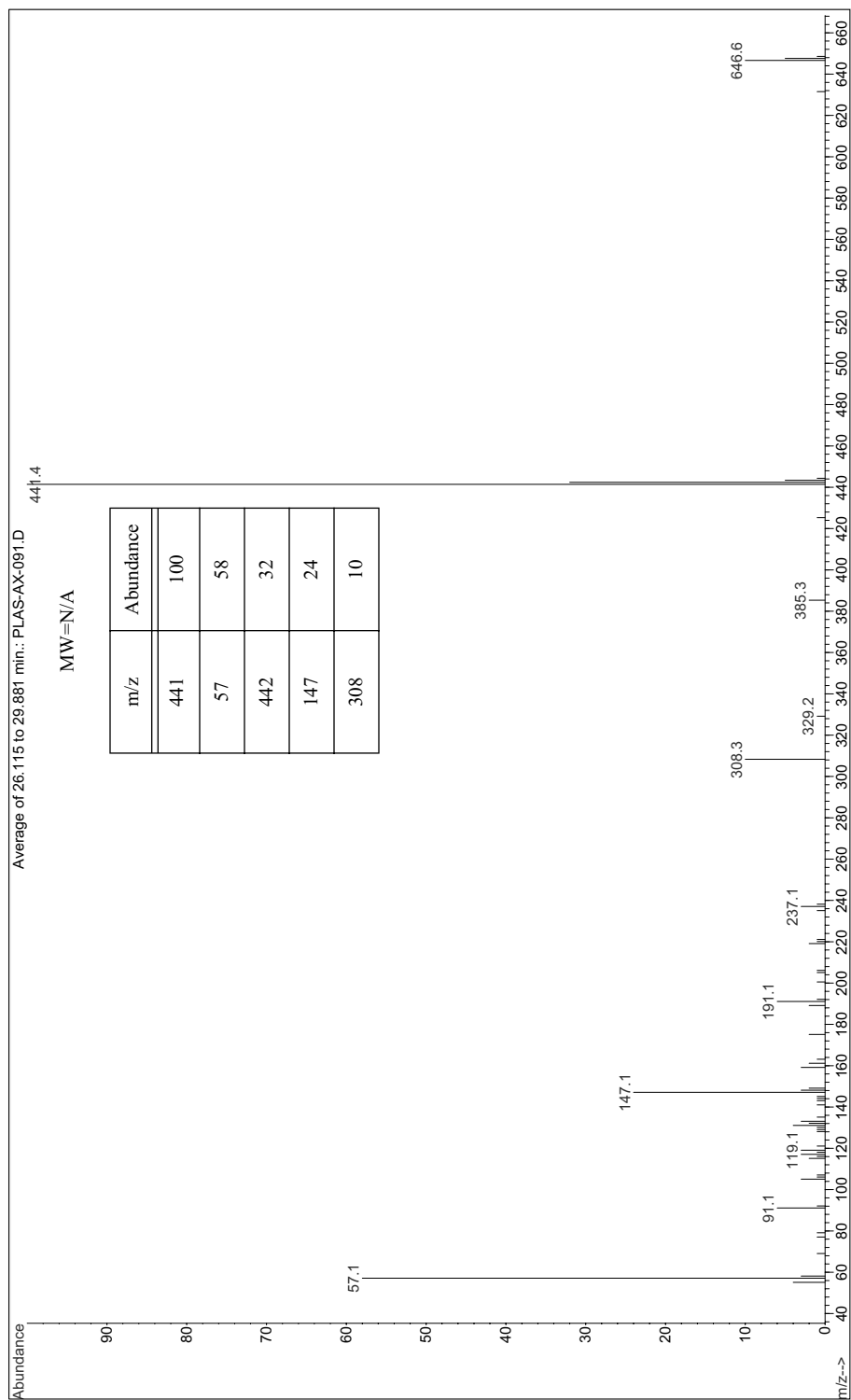
For Chromatogram See Appendix A - PLAS-AX-091 - page 468

Mass Spectrum for *BNX 1225 TPR - PLAS-AX-091*

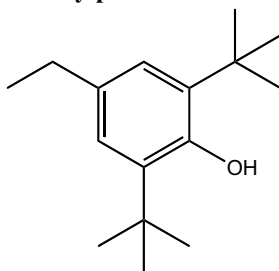


For Chromatogram See Appendix A - PLAS-AX-091 - page 468

Mass Spectrum for *BNX 1225 TPR - PLAS-AX-091*



For Chromatogram See Appendix A - PLAS-AX-091 - page 468

2,6-Di-tert-butyl-4-ethylphenol

CAS Number 4130-42-1
RTECS Number N/A
Abbreviation DBEP

Formula C₁₆H₂₆O
Molecular Weight 234.38

Chemical Name

2,6-ditert-butyl-4-ethylphenol

Synonyms

2,6-bis(1,1-dimethylethyl)-4-ethylphenol

Brand Names & Manufacturers

Antioxidant DBEP

Sandant 425

Yoshinox 250

Xiangshui Fumei Chemical Co., Ltd.

Physical Properties**Appearance** Light Yellow liquid**Melting Point** >44 °C**Boiling Point** 272 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application A hindered phenol antioxidant used in plastics and rubber products to impart excellent high temperature stability and discoloration resistance. It can be used in combination with phosphites, thioesters, and other antioxidants.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Based on its physical and chemical properties as well as empirical biodegradation data, DBEP is not expected to degrade quickly in the environment. It is persistent in water, soil, and sediments. It also has the potential to accumulate in organisms and may biomagnify in food chains. The substance has been determined to meet the persistence and bioaccumulation criteria. In addition, aquatic toxicity data indicate that the substance is potentially highly hazardous to aquatic organisms.

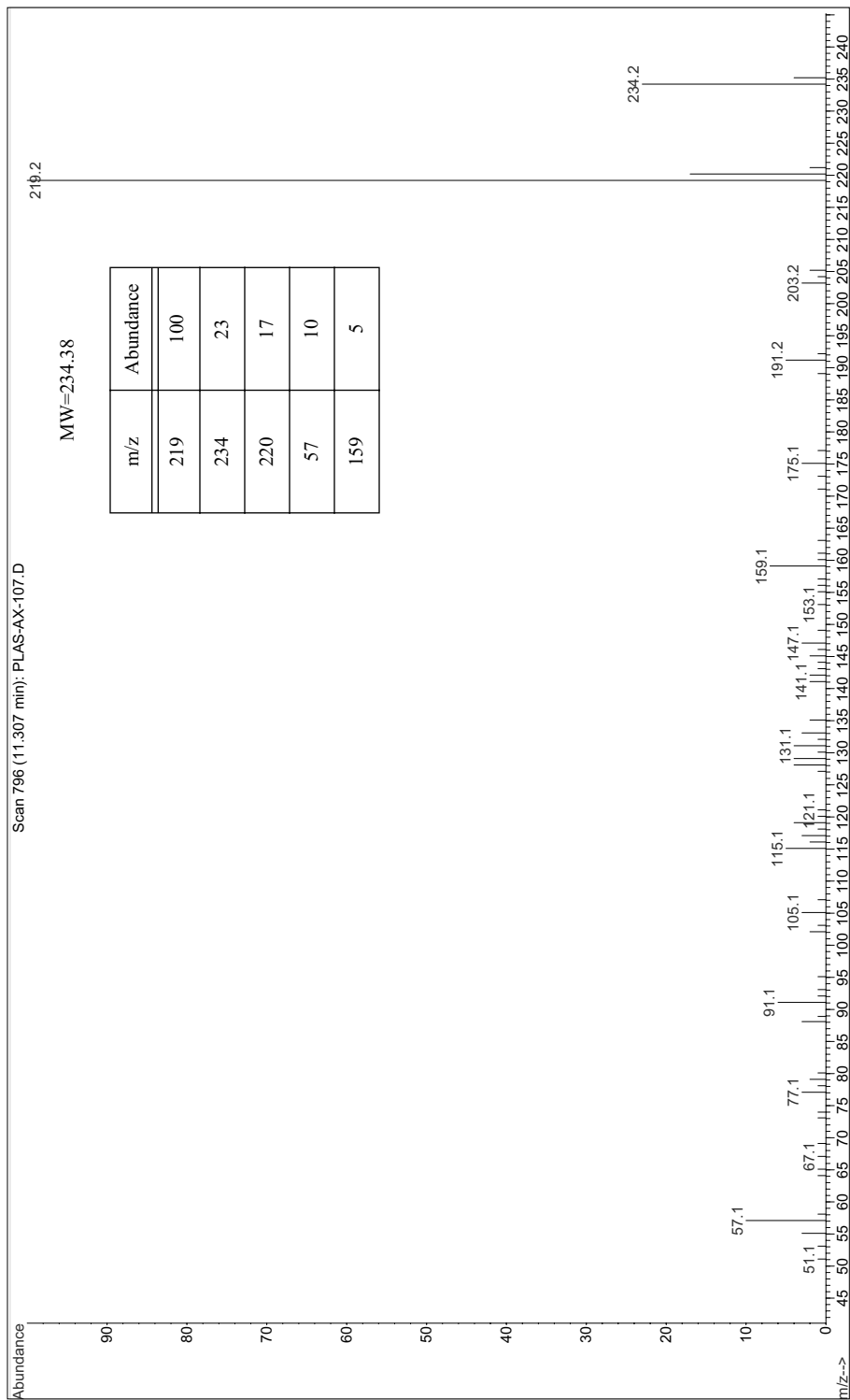
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

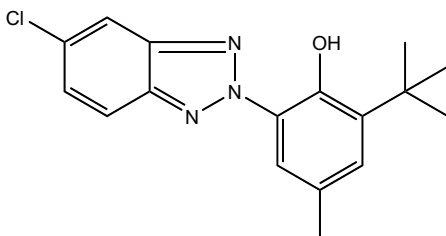
Toxicological Data

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Mass Spectrum for 2,6-Di-tert-butyl-4-ethylphenol - PLAS-AX-107



For Chromatogram See Appendix A - PLAS-AX-107 - page 469

2-tert-butyl-6-(5-chlorobenzotriazol-2-yl)-4-methylphenol**CAS Number** 3896-11-5**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₁₇H₁₈ClN₃O**Molecular Weight** 315.80**Chemical Name**

2-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)-4-methylphenol

Synonyms

2-(3-tert-butyl-2-hydroxy-5-methylphenyl)-5-chloro-2h-benzotriazole; 2-(5-chloro-2-benzotriazolyl)-6-tert-butyl-p-cresol

Brand Names & ManufacturersBLS® 1326
Tinuvin® 326Mayzo
Ciba**Physical Properties****Appearance** Slightly yellowish powder**Melting Point** 138-141 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.1	0.1	1	4.3	1.0

Application, Regulatory & Environmental Information**Application**
Protects polymers from UV radiation helping to preserve the original appearance and physical integrity, especially for polyolefins and polyester resins.**Regulatory Information**

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body. Approved for indirect food contact in polyolefins.

Environmental Impact

LC50: 100 mg/L - 96 h [Fish]

EC50: 100 mg/L - 24 h [Daphnia magna (Water flea)]

EC50: 100 mg/L - 72 h [Algae]

According to the results of tests of biodegradability this product is not readily biodegradable.

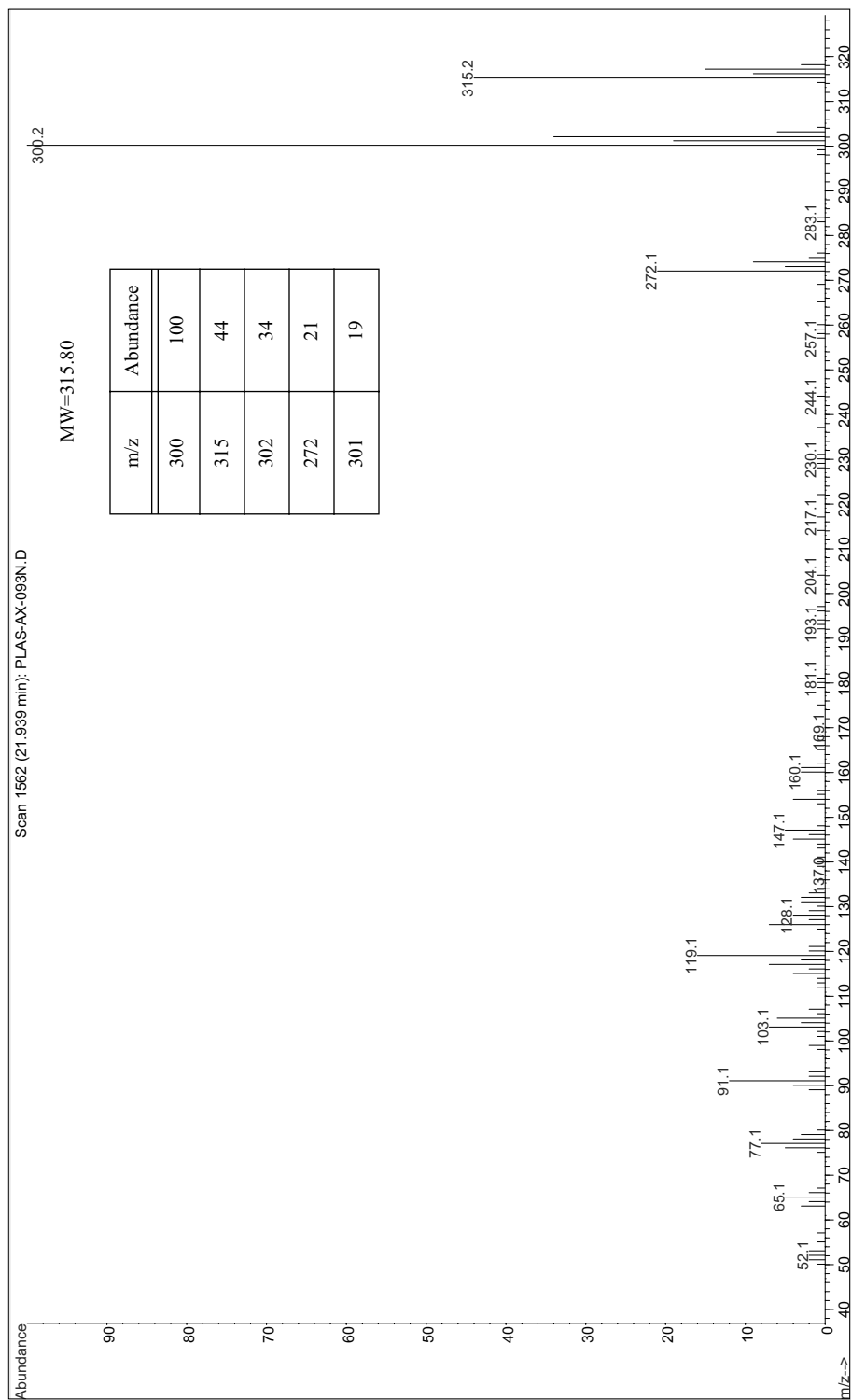
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

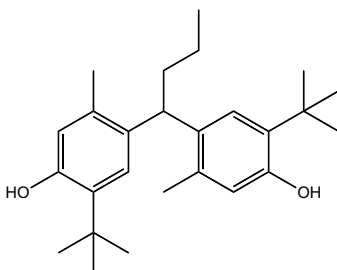
Toxicological Data

Oral LD50: 5000 mg/kg [Rat]

Mass Spectrum for 2-tert-butyl-6-(5-chlorobenzotriazol-2-yl)-4-methylphenol - PLAS-AX-093



For Chromatogram See Appendix A - PLAS-AX-093 - page 470

4,4'-Butylenedibis(6-tert-butyl-m-cresol)**CAS Number** 85-60-9**RTECS Number** GO7050000**Abbreviation** BBMC**Formula** C₂₆H₃₈O₂**Molecular Weight** 382.58**Chemical Name**

4,4'-butane-1,1'-diylbis(2-tert-butyl-5-methylphenol)

Synonyms

6,6'-di-tert-butyl-4,4'-butylenedi-m-cresol

Brand Names & Manufacturers

Lowinox® 44B25

Chemtura

Santowhite®

Monsanto

Sumilizer BBM

Sumitomo Chemical

Physical Properties**Appearance** Translucent pellets**Melting Point** 209 °C**Boiling Point** 472 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	43	43	>200	U	U

Application, Regulatory & Environmental Information**Application**

A commercial antioxidant used in the manufacture of polypropylene. Suitable for the protection of white and light-colored compounds and in paper coatings applications. It provides good UV stability and resistance to attack by NO_x (nitrogen oxides).

Regulatory Information

FDA 21CFR §175.105 (Indirect food additives), §175.210, §175.300, §177.1632, §177.2600 §178.2010. BgWXXI compliant; CERCLA nonreportable; DOT, IATA not regulated. TSCA listed.

Environmental Impact

LC50 (96 hour): > 1000 mg/L [Rainbow trout]

LC50 (96 hour): > 1000 mg/L [Bluegil sunfish]

LC50 (96 hour): > 1000 mg/L [Fatheadminnow]

EC50 (96 hour): > 1000 mg/L [Algae]

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

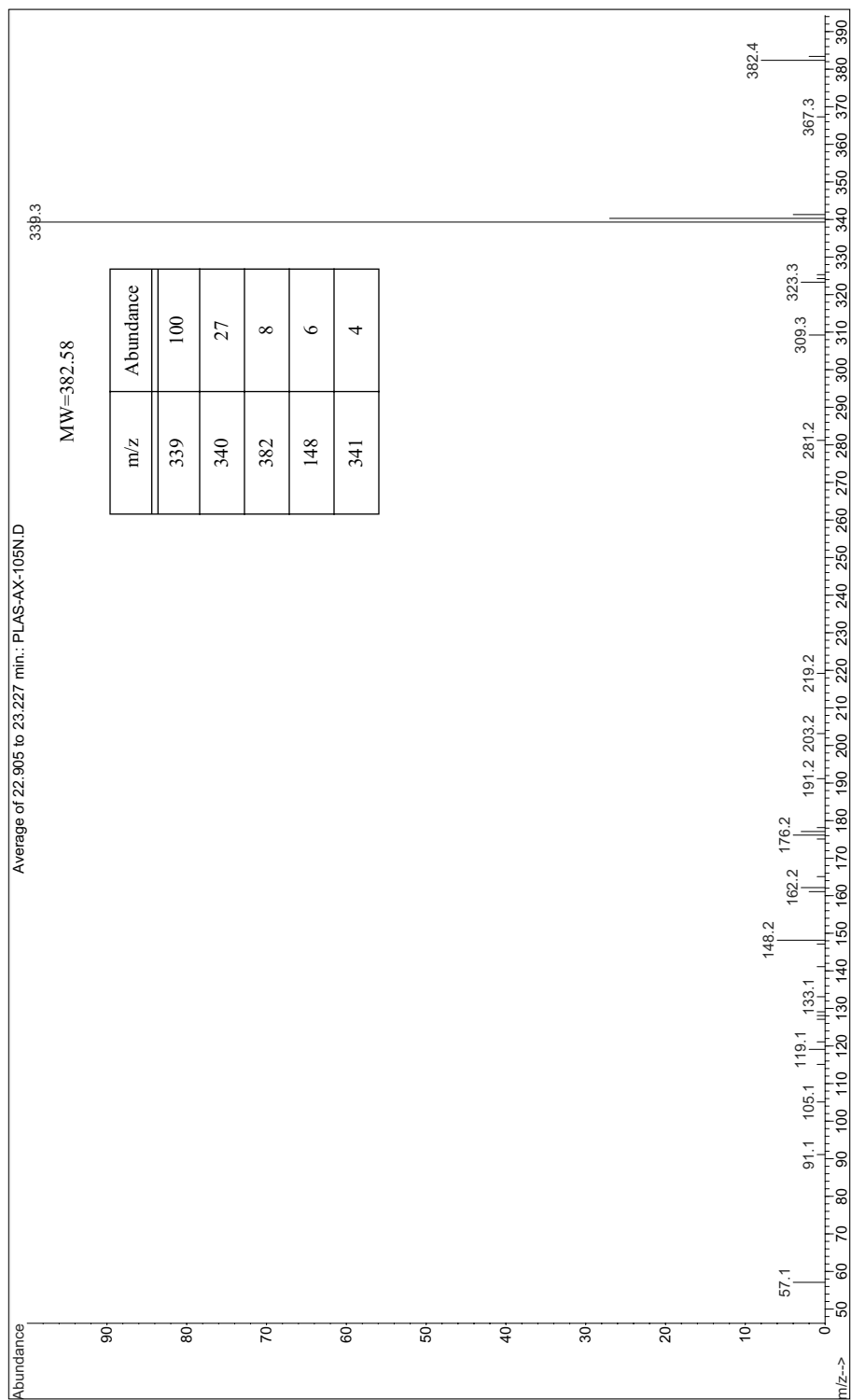
Toxicological Data

Oral LDLo (Lowest published lethal dose): 17 gm/kg [Rat]

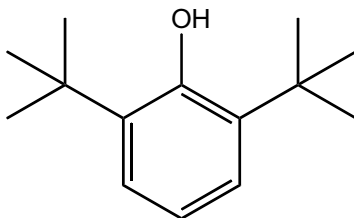
Oral TDLo (Lowest published toxic dose): 1824 mg/kg/1W-C [Rat]

LD50 (dermal): >7940 mg/kg

Mass Spectrum for 4,4'-Butylidenebis(6-tert-butyl-m-cresol) - PLAS-AX-105



For Chromatogram See Appendix A - PLAS-AX-105 - page 471

2,6-Di-tert-butylphenol**CAS Number** 128-39-2**RTECS Number** SK8265000**Abbreviation** 2,6-DTBP**Formula** C₁₄H₂₂O**Molecular Weight** 206.32**Chemical Name**

2,6-ditert-butylphenol

Synonyms

2,6-ditert-butylphenol

Brand Names & ManufacturersEthanox[®] 701Isonox[®] 103**Physical Properties****Appearance** White crystals**Melting Point** 34-36 °C**Boiling Point** 253 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.04	S	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Used industrially as UV stabilizer and an antioxidant for hydrocarbon-based products ranging from petrochemicals to plastics.

Regulatory Information

This substance is designated by the U.S. Department of Transportation (DOT) as a marine pollutant.

Environmental Impact

This substance is highly toxic to aquatic organisms and has been assigned a Water Hazard Classification under the June 1999 Administrative Regulation on Substances Hazardous to Waters. Bioaccumulation may occur.

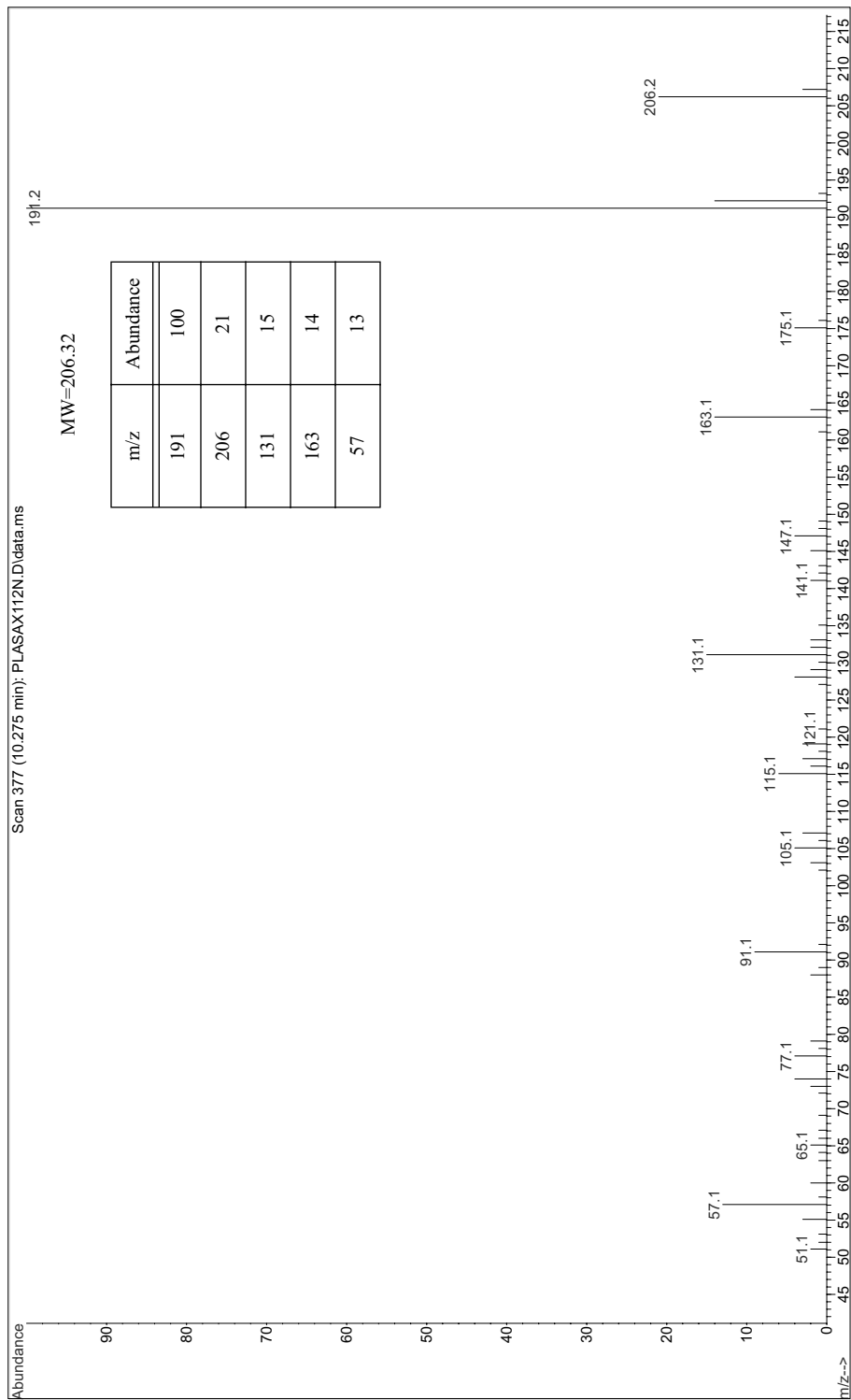
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

LD50: 9200 mg/kg

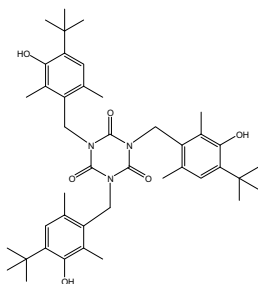
Mass Spectrum for 2,6-Di-tert-butylphenol - PLAS-AX-112



For Chromatogram See Appendix A - PLAS-AX-112 - page 472

Cyanox® 1790

Cytex Technology Corporation

**CAS Number** 4061-76-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₄₂H₅₇N₃O₆**Molecular Weight** 699.92**Chemical Name**

1,3,5-tris(4-tert-butyl-3-hydroxy-2,6-dimethylbenzyl)-1,3,5-triazine-2,4,6-(1h, 3h,5h)-trione

Synonyms

N/A

Brand Names & Manufacturers

Lowinox® 1790

Chemtura Corporation

Physical Properties**Appearance** White powder**Melting Point** 159-162 °C**Boiling Point** >300 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 1.4	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Used for polyurethane, polypropylene, polyester, and polyamide fibers where it provides fading resistance at low load levels. In addition, the molecular structure and the relatively high molecular weight results in a high extraction resistance in demanding applications like hot water polypropylene pipes.

Regulatory Information

Cyanox® 1790 is approved as an antioxidant at levels not to exceed 0.1% in olefin polymers used in the manufacture of articles that contact food, subject to the provisions of 21CFR178.2010(b) of the Food Additives Regulations, and is approved for use in polystyrene and rubber-modified polystyrene under 21CFR177.1640.

Environmental Impact

This substance is not readily biodegradable and has a log Kow value of 15.281, which would indicate a potential to bioaccumulate. This substance is not expected to be hazardous to aquatic substances due to its limited solubility in water.

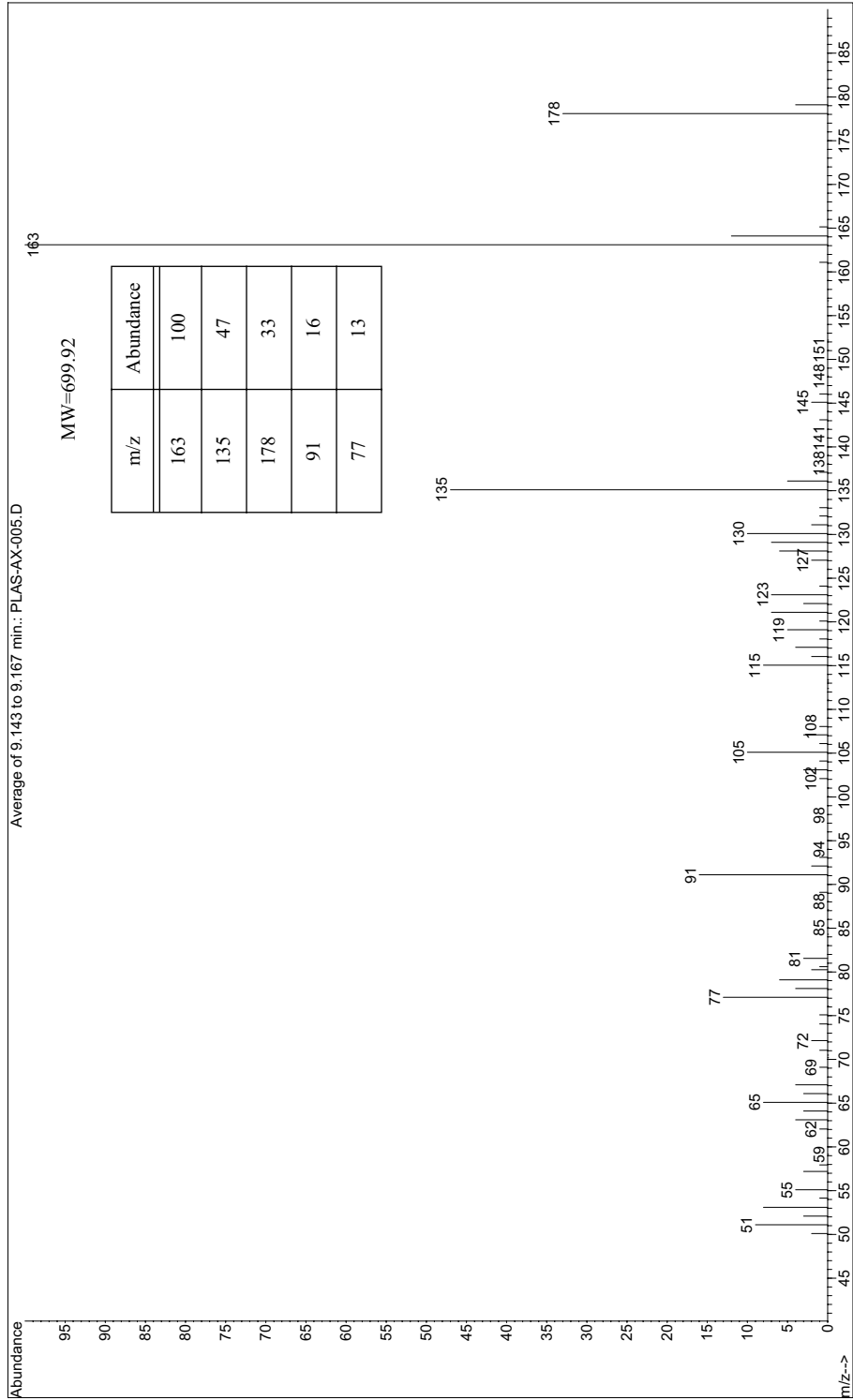
Point of Release

Capable of transferring constituents of the additive into food substances.

Toxicological Data

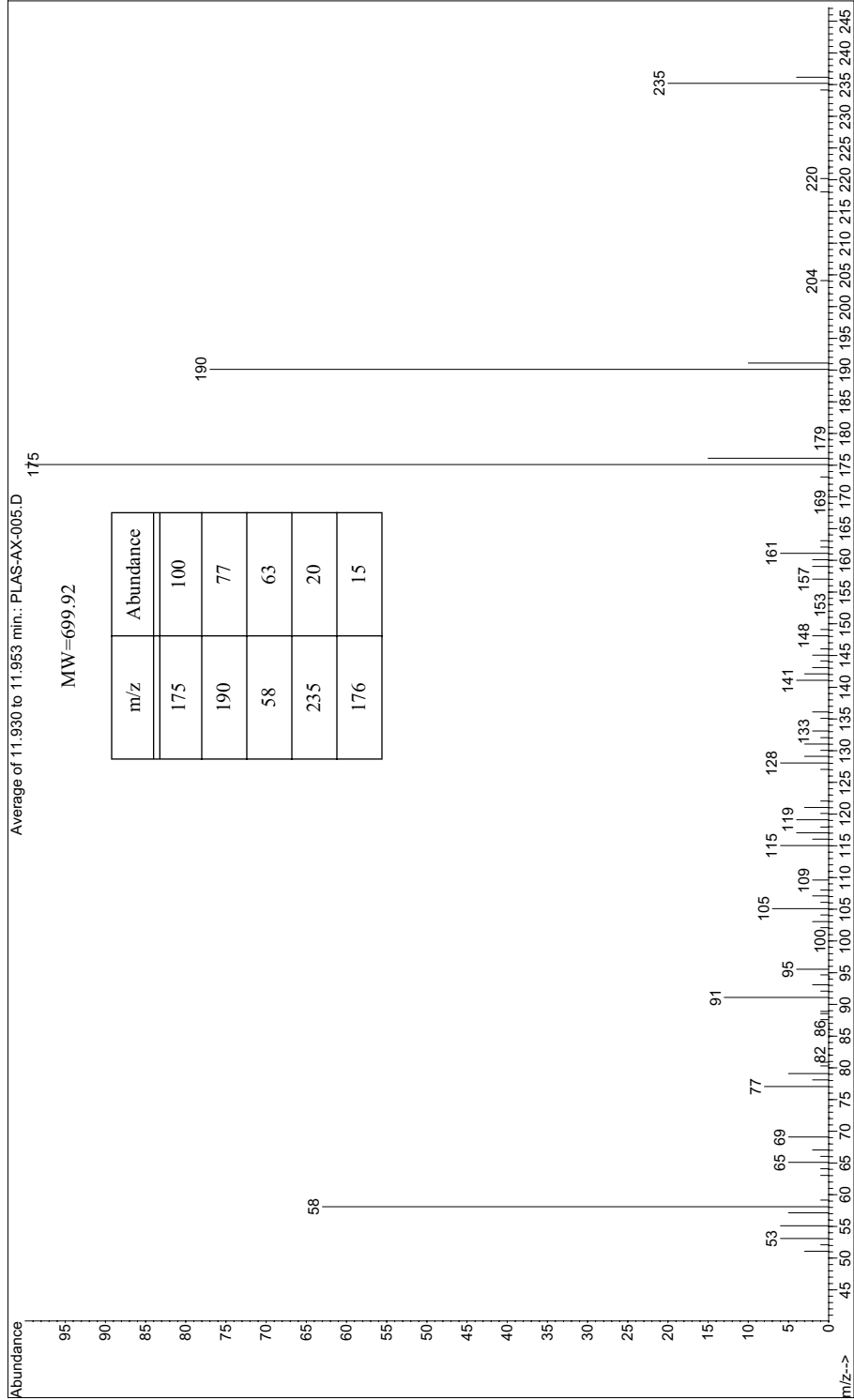
Acute oral (LD50): >10,000 mg/kg [Rat], >5000 mg/kg [Rabbit].

Mass Spectrum for Cyanox® 1790 - PLAS-AX-005



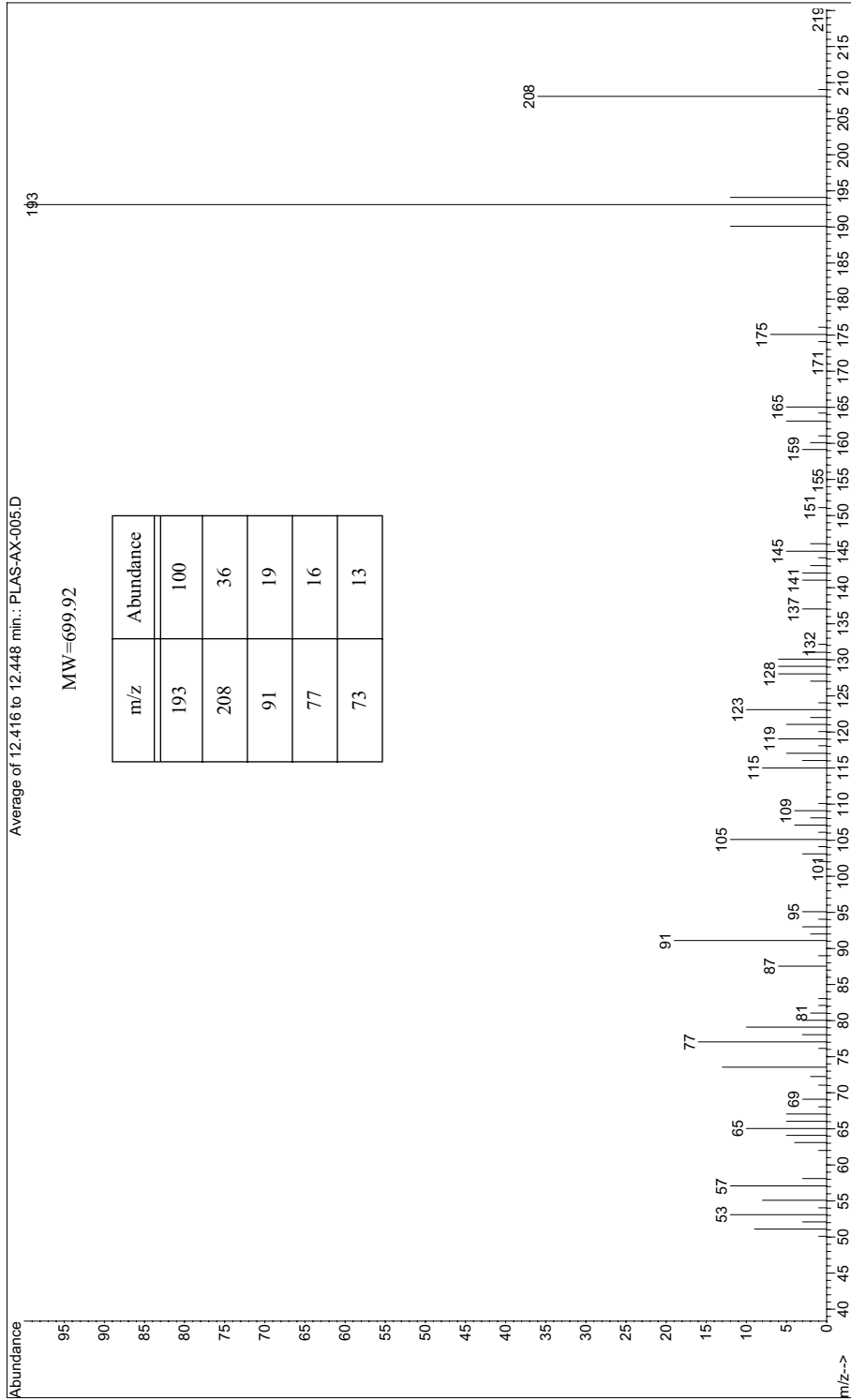
For Chromatogram See Appendix A - PLAS-AX-005 - page 473

Mass Spectrum for Cyanox[®] 1790 - PLAS-AX-005



For Chromatogram See Appendix A - PLAS-AX-005 - page 473

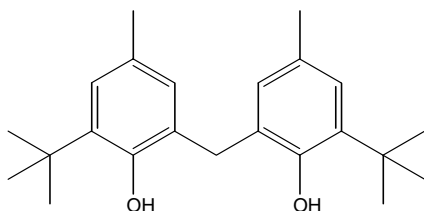
Mass Spectrum for Cyanox® 1790 - PLAS-AX-005



For Chromatogram See Appendix A - PLAS-AX-005 - page 473

Cyanox[®] 2246

Cytec Technology Corporation

**CAS Number** 119-47-1**RTECS Number** PA3500000**Abbreviation** Not Identified**Formula** C₂₃H₃₂O₂**Molecular Weight** 340.55**Chemical Name**

2,2'-methylene-bis-(4-methyl-6-tert-butyl-phenol)

Synonyms

bis(2-hydroxy-3-tert-butyl-5-methylphenyl)methane; 2,2'-methylenebis(6-tert-butyl-4-methylphenol); 2,2'-methylenebis(6-tert-butyl-p-cresol)

Brand Names & Manufacturers

Advastab [®]	Rohm and Haas Chemicals LLC
Lowinox [®] 22M46	Chemtura Corporation
Antioxidant 235	Akrochem Corporation
Plastanox [®] 2246	American Cyanamid Corp

Physical Properties

Appearance	White crystalline powder, faint phenolic odor					
Melting Point	127-129 °C			Boiling Point	Not available	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH 154	Acetone 175	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application
Used as a thermo/light-stabilizing phenolic antioxidant in the manufacture (compounding and end use) of white, light-colored, and transparent vulcanizates based on natural or synthetic rubber, PS, polyolefins, and pentaplast. Also used in POM and ABS thermoplastics because of its low volatility and migration properties.

Regulatory Information

FDA approved 1998: olefin polymer material in contact with food, not to exceed 0.1% w/w; POM copolymers, not to exceed 1.0% w/w; POM homopolymers, not to exceed 0.5% w/w. 21 CFR allows for the use in all stages of production, processing, and packaging of food for the following applications: 21CFR175.105 use in adhesives, 21CFR177.2600 manufacturing rubber material, and 21CFR178.2010 manufacturing antioxidants/stabilizers.

Environmental Impact

(LC50): > 100 mg/L [*Leuciscus idus*] (LC50 96 hour): > 50 mg/L [Fish], (EC50 3 hour): >10 g/L [Bacteria]. No effects observed in tests on *Pseudomonas putida* and *E. coli*.

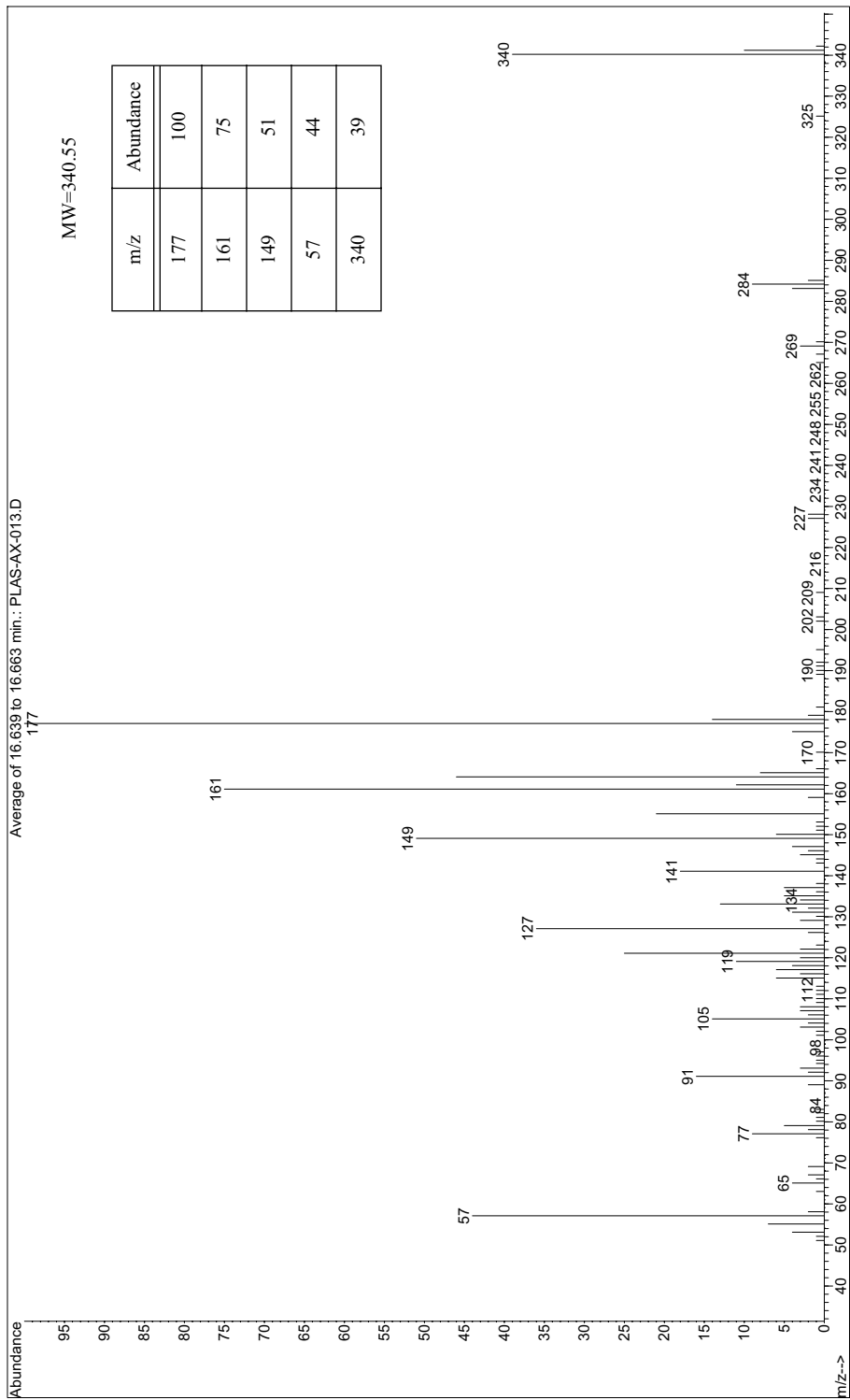
Point of Release

The compound possesses low volatility and migration.

Toxicological Data

The toxicological properties of this material have not been thoroughly investigated. Not listed (ACGIH, IARC, NTP, OSHA) as a cancer-causing agent. Acute oral (LD50): >10 g/kg [Rat]; acute dermal (LD50): >10 g/kg [Rabbit].

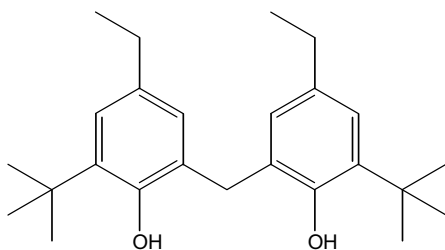
Mass Spectrum for Cyanox® 2246 - PLAS-AX-013



For Chromatogram See Appendix A - PLAS-AX-013 - page 474

Cyanox[®] 425

Cytec Technology Corporation

**CAS Number** 88-24-4**RTECS Number** SL9800000**Abbreviation** Not Identified**Formula** C₂₅H₃₆O₂**Molecular Weight** 368.55**Chemical Name**

2,2'-methylenebis(4-ethyl-6-tert-butylphenol)

Synonyms

2,2'-methylenebis(6-tert-butyl-4-ethylphenol)

Brand Names & Manufacturers

Cyanox 425

Cytec Technology Corporation

Physical Properties**Appearance** Cream-colored free-flowing powder**Melting Point** 117-129 °C**Boiling Point**

Decomposes

Stability Stable under normal conditions of use.**Solubility**
(g/100mL 20 °C)**Water**
<0.1**MeOH**
U**EtOH**
U**Acetone**
U**CH₂Cl₂**
U**Hexane**
U**Application****Application, Regulatory & Environmental Information**

Cyanox[®] 425 is a bisphenol compound recommended for use in rubber modified plastics and is effective in the stabilization of ABS.

Regulatory Information

FDA approved under 21CFR178.2010 for use in acrylonitrile-butadiene-styrene copolymers at levels not to exceed 0.6% by weight of the copolymer. Section 177.1010 for use in semi-rigid and rigid acrylics at levels not to exceed 0.1% by weight of the plastic, and Section 175.105 as a component of food packaging adhesives. Also, approved by the FDA as an antioxidant in the preparation of rubber articles at a level not to exceed 5% by 21CFR177.2600.

Environmental Impact

Due to extreme low solubility in water, and therefore the non-availability to species, this product is regarded as not hazardous to aquatic organisms. The product is also not readily biodegradable, and potential bio-accumulation could occur, based on the molecular structure and the calculated log Pow.

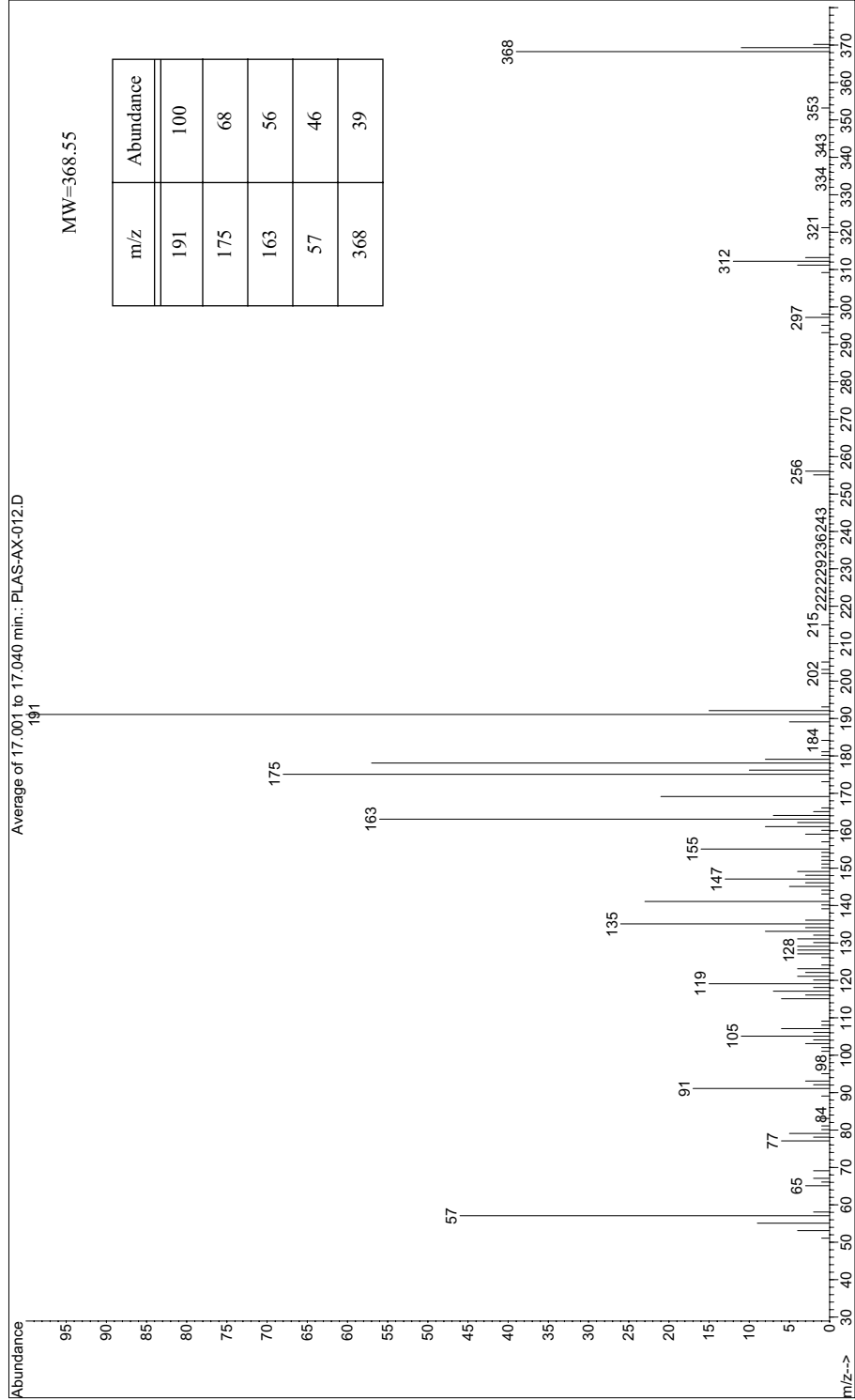
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Reproductive Effector. Acute oral toxicity (LD50): >10 gm/kg [Rat], lowest published toxic oral dose (TDLo): 80 gm/kg/12W-C [Rat].

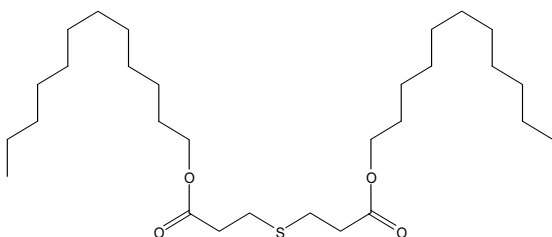
Mass Spectrum for Cyanox[®] 425 - PLAS-AX-012



For Chromatogram See Appendix A - PLAS-AX-012 - page 475

Cyanox[®] LTDP

Cytec Technology Corporation

**CAS Number** 123-28-4**RTECS Number** UF8000000**Abbreviation** LTDP**Formula** C₃₀H₅₈O₄S**Molecular Weight** 514.85**Chemical Name**

dilaurylthiopropionate

Synonyms

di-lauryl-3,3'-thiodipropionate; 3,3'-thiodipropionic acid, didodecyl ester; didodecyl-3,3'-thiopropionate

Brand Names & ManufacturersAdvastab[®] 800Lowinox[®] DLTDPNaugard[®] DLTDP

Rohm and Haas Chemicals LLC

Chemtura Corporation

Chemtura Corporation

Physical Properties

Appearance	White crystalline powder, characteristic sweet odor					
Melting Point	38-41 °C		Boiling Point		Not available	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH <0.01	Acetone U	CH₂Cl₂ U	Hexane U

Application**Application, Regulatory & Environmental Information**

LTDP is a thiosynergist antioxidant additive to thermo/light-stabilizers (used in combination with phenolic antioxidants) with plasticizing properties used to decompose and neutralize hydroperoxides, formed by the auto-oxidation of polymers, primarily in PE, PP, ABS, polyester, and polyamide.

Regulatory Information

FDA approved 1998 for the manufacture of resinous/polymeric coatings in safe contact with food for articles for use in all stages of production, processing, packaging, and transport of food, 21CFR175.300. Joint FAO/WHO committee on Food Additives recommended an ADI of 3.0 mg/kg BW. Inventories: AICS (Australia); DSL (Canada); ECL (Korea); EINECS (Europe); ENCS (Japan); List I (China); PICCS (Philippines); TSCA (US).

Environmental Impact

(LC50 96 hour): 71 mg/L [Fish], (EC50 24 hour): 10 mg/L [Daphnia], (EbC 72 hour): 33.9 mg/L [Algae].

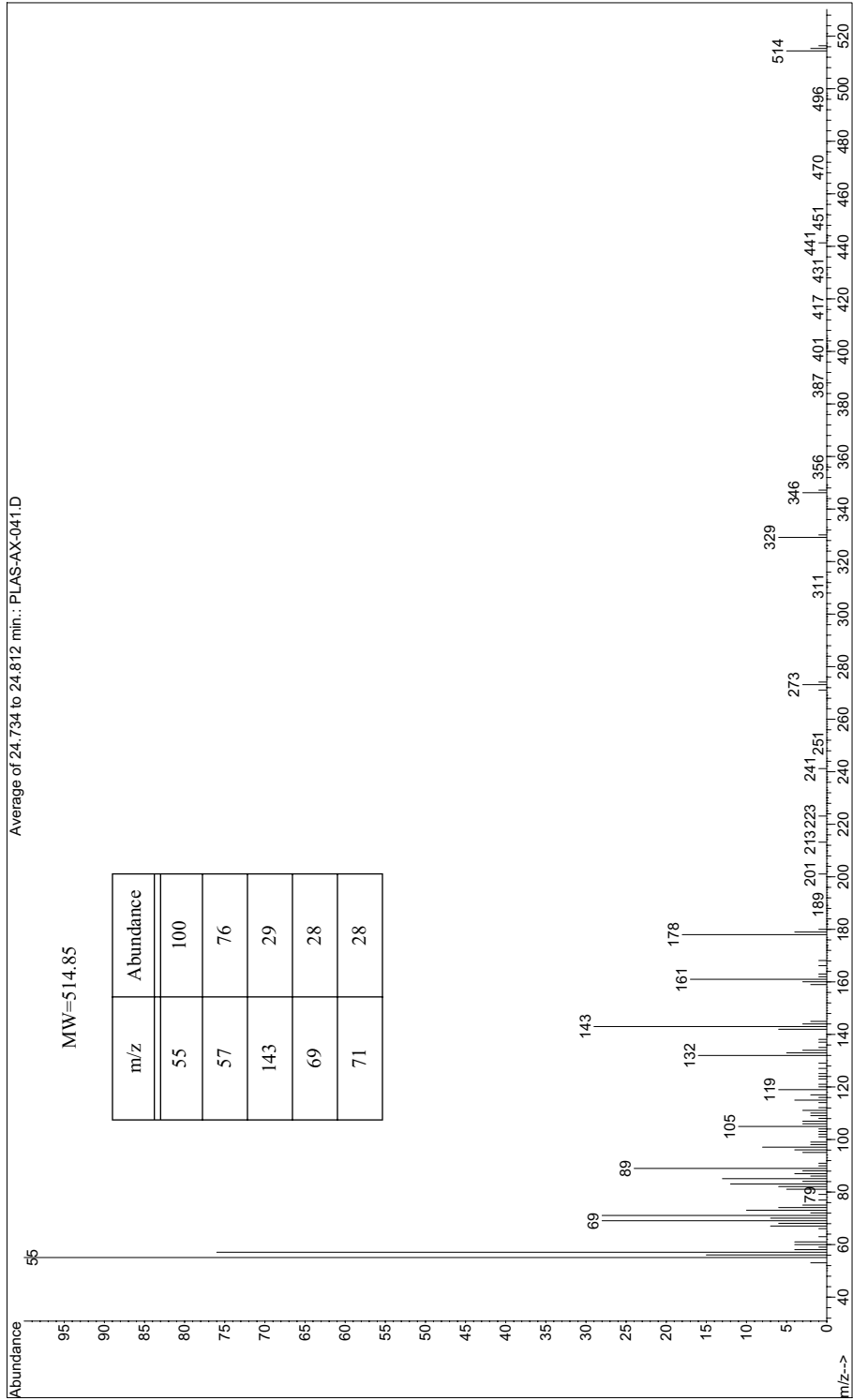
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed by ACGIH, IARC, NTP, or OSHA as a cancer-causing agent. The toxicological properties of this material have not been thoroughly investigated. Acute inhalation (4 hour) (LC50): >3000 ppm [Rat], acute intraperitoneal (LD50) >2 g/kg [Mouse], acute oral (LD50): >2 g/kg [Mouse], >25 g/kg [Rat], acute dermal (LD50): >10 g/kg [Rabbit]. Long-term toxicological effect of growth-retardation in rats fed 1 and 3% LTDP over 2 years, no changes in visceral organs reported.

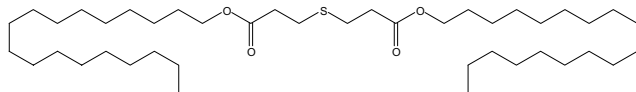
Mass Spectrum for Cyanox[®] LTDP - PLAS-AX-041



For Chromatogram See Appendix A - PLAS-AX-041 - page 476

Cyanox[®] STDP

Cytec Technology Corporation

**CAS Number** 693-36-7**RTECS Number** UF8010000**Abbreviation** DSTDP**Formula** C₄₂H₈₂O₄S**Molecular Weight** 683.30**Chemical Name**

distearylthiopropionate

Synonyms

distearyl-3,3'-thiodipropionate; thiodipropionic acid, dioctodecyl ester; distearyl beta-thiodipropionate

Brand Names & ManufacturersAdvastab[®] 802Lowinox[®] DSTDPNaugard[®] DSTDP

Rohm and Haas Chemicals, LLC

Chemtura Corporation

Chemtura Corporation

Physical Properties**Appearance** White crystalline powder**Melting Point** 63-67 °C**Boiling Point** ~658 °C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<0.01	<0.01	U	S	S

Application, Regulatory & Environmental Information**Application**

STDP is a thiosynergist antioxidant additive to thermo/light-stabilizers (used in combination with phenolic antioxidants) with plasticizing properties used to decompose and neutralize hydroperoxides, formed by the auto-oxidation of polymers, primarily in PE, PP, ABS, polyester, and polyamide.

Regulatory Information

FDA approved 1998 use of STDP in the manufacture of resinous/polymeric coatings in safe contact with food for articles for use in all stages of production, processing, packaging, and transport of food, 21CFR175.300.

Environmental Impact

Inherently biodegradable OECD 302C: 60%. Log Kow 17.68 (estimated). Hydrolysis >2 years. Toxicity to aquatic biota: (LC50 96 hour): >100 mg/L [Fish; (EC50 24 hour): 780 mg/L [Daphnia]; EbC50 (72 hour): 60 mg/L [Algae].

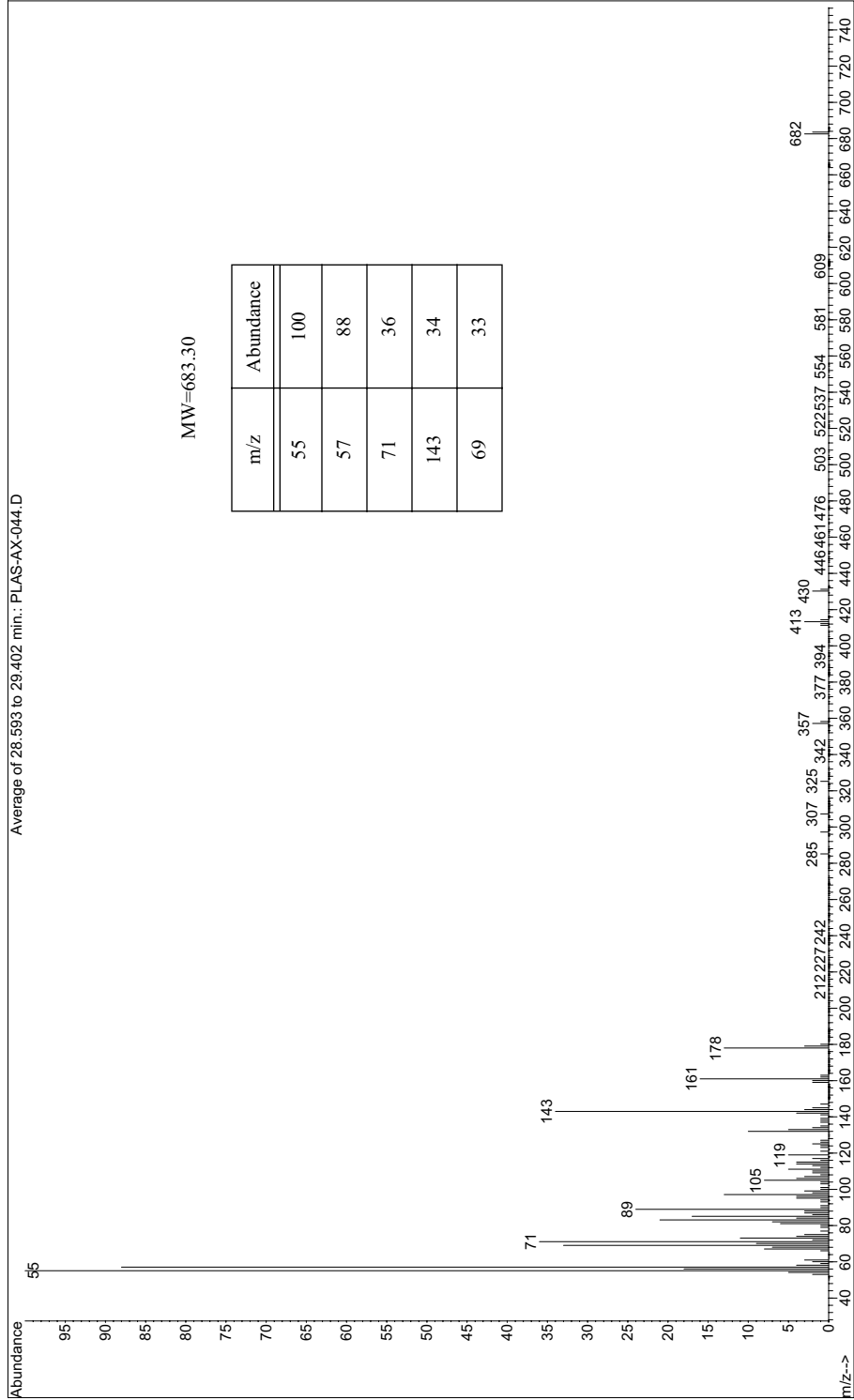
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

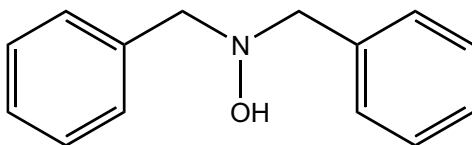
Toxicological Data

Long-term toxicological effect of BW growth-retardation in rats fed 3% LTDP in their diet over 2 years — no changes in visceral organs reported. Not determined to be carcinogenic (NTP, IARC, OSHA, ACGIH). Acute oral LD50: > 5 g/kg [Rat]. Acute dermal LD50: > 2 g/kg [Rabbit].

Mass Spectrum for Cyanox® STDP - PLAS-AX-044



For Chromatogram See Appendix A - PLAS-AX-044 - page 477

Dibenzylhydroxylamine**CAS Number** 621-07-8**RTECS Number** N/A**Abbreviation** DBHA**Formula** C₁₄H₁₅NO**Molecular Weight** 213.28**Chemical Name**

N,N-dibenzylhydroxylamine

Synonyms

N/A

Brand Names & Manufacturers

Antioxidant DBHA

Mizat

BNX[®] 2000

Mayzo

Physical Properties**Appearance** White powder**Melting Point** 125-128 °C**Boiling Point** 379.7 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	U	U	U	U

Application *Application, Regulatory & Environmental Information*

Typical end use applications include textiles and fibers, particularly as an anti-yellowing agent for elastomeric nylons (i.e., spandex or lycra). In addition, it can be used in polyolefin systems where fading or phenolic yellowing is known to occur.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

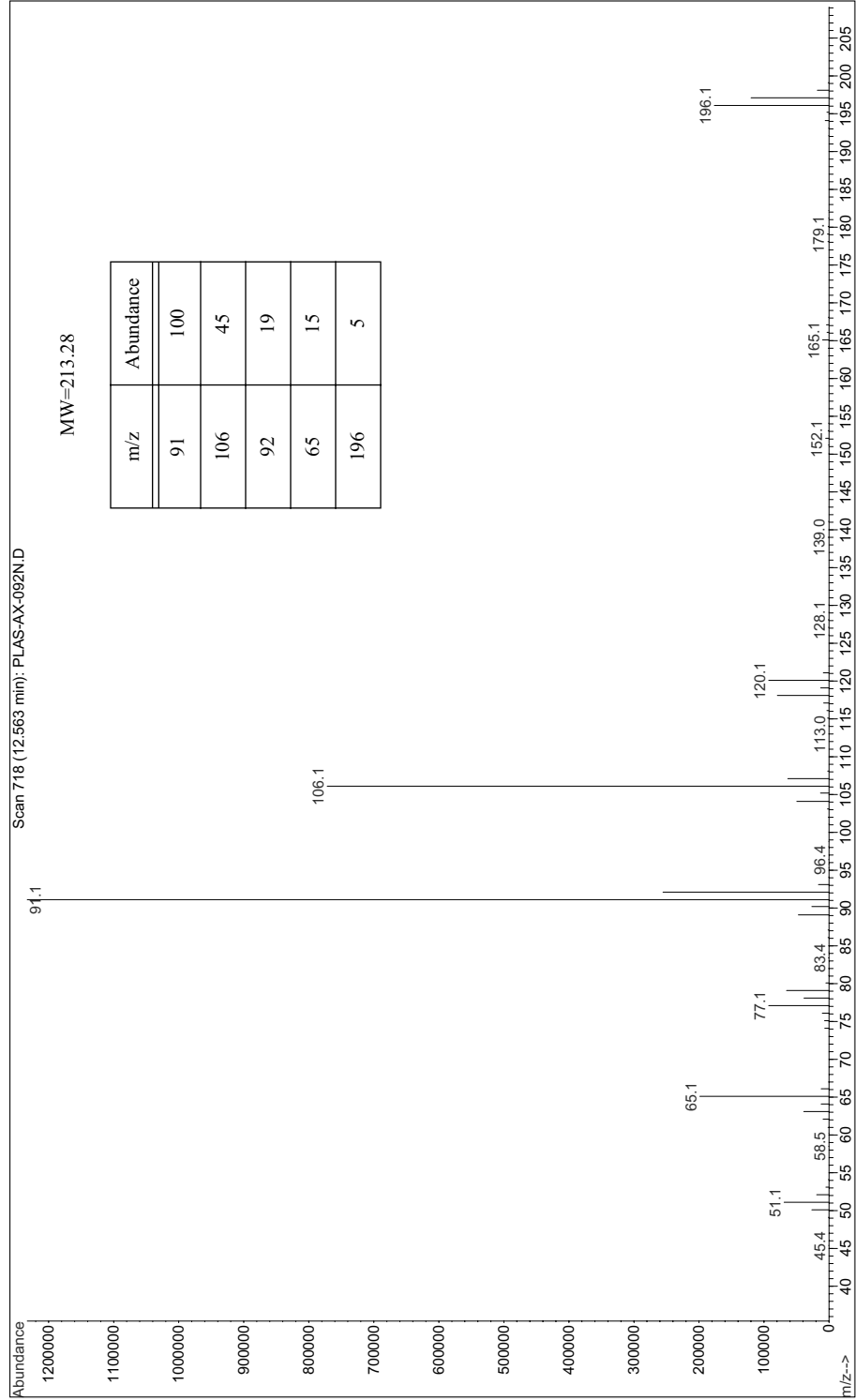
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

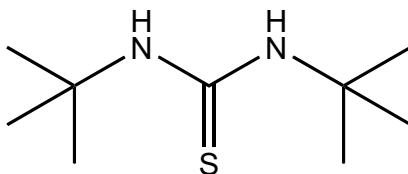
Toxicological Data

Toxicological effects are unknown. Repeated and prolonged exposure to this product is not known to aggravate existing medical conditions.

Mass Spectrum for Dibenzylhydroxylamine - PLAS-AX-092



For Chromatogram See Appendix A - PLAS-AX-092 - page 478

N,N'-Dibutylthiourea**CAS Number** 109-46-6**RTECS Number** YS8400000**Abbreviation** DBTU**Formula** C₉H₂₀N₂S**Molecular Weight** 188.33**Chemical Name**

1,3-dibutylthiourea

Synonyms

N/A

Brand Names & Manufacturers

Ekaland DBTU

Thiate® U

Westco DBTU

Westco DBTU

RT Vanderbilt

Western Reserve Chemical

Physical Properties**Appearance** White to light yellow powder**Melting Point** 63-67 °C**Boiling Point** 122 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	S	U	S	U	U

Application, Regulatory & Environmental Information**Application**

N,N'-Dibutylthiourea is a nitrosamine free accelerator, antidegradant, and corrosion inhibitor. Ultra-accelerator for mercaptan-modified CR. It is slightly safer than DETU. It is also used as a secondary accelerator for NR and synthetic rubbers. It disperses easily in rubber. It is non-staining and does not bloom. It is practically odorless. Antioxidant for NR, antiozonant for NR and SR, particularly SBR.

Regulatory Information

Regulated for use under 21 CFR §177.2600 Rubber Articles Intended for Repeated Use in Food Contact.

Environmental Impact

LC50: 10.7 mg/l - 48 h [Daphnia magna (Water flea)]

Point of Release

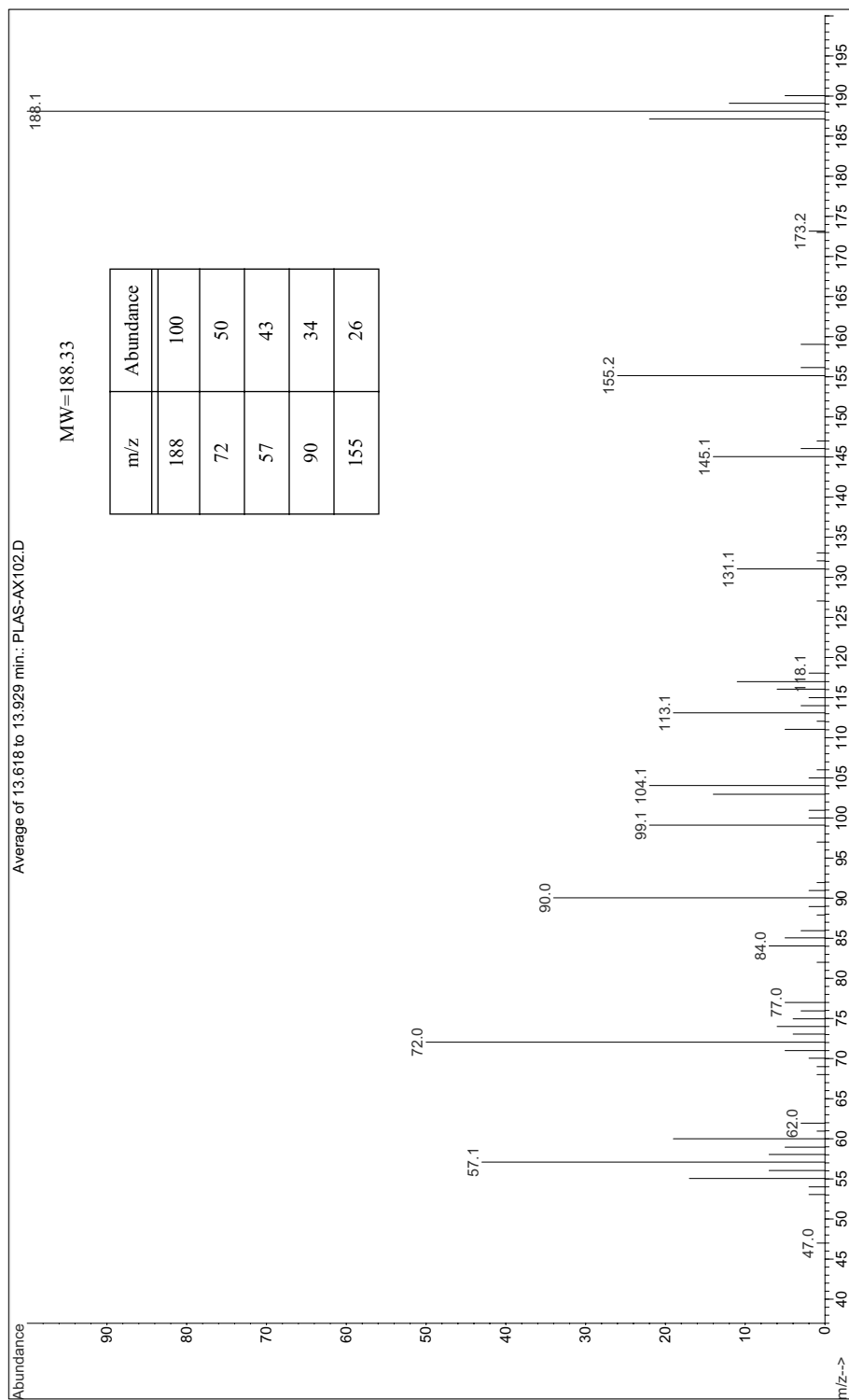
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

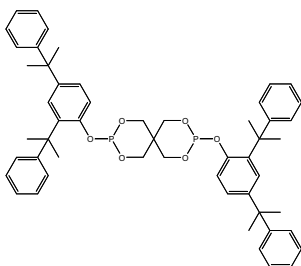
Acute oral (LD50): >350 mg/kg [Rat]

Acute dermal (LD50): >2000 mg/kg [Rabbit]

Mass Spectrum for N,N'-Dibutylthiourea - PLAS-AX-102



For Chromatogram See Appendix A - PLAS-AX-102 - page 479

3,9-Bis(2,4-dicumylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane**CAS Number** 154862-43-8**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₅₃H₅₈O₆P₂**Molecular Weight** 852.97**Chemical Name**

3,9-bis[2,4-bis(2-phenylpropan-2-yl)phenoxy]-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane

Synonyms

2,4,8,10-tetraoxa-3,9-diphosphaspiro(5.5)undecane, 3,9-bis(2,4-bis(1-methyl-1-phenylethyl)phenoxy)-

Brand Names & ManufacturersAlkanox[®] 28Doverphos[®] S-9228

Chemtura

Dover Chemical Company

Physical Properties**Appearance** White to off-white powder**Melting Point** 229-232 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	U	U	U	U

Application, Regulatory & Environmental Information

Application Free-flowing solid phosphite secondary antioxidant used in adhesives. Excellent hydrolytic stability in addition to excellent in polymer melt flow and color stability. Because of its high melting point, it can be utilized in applications that require processing at elevated temperatures.

Regulatory Information

FDA approved for indirect food contact 21CFR §178.2010.

Environmental Impact

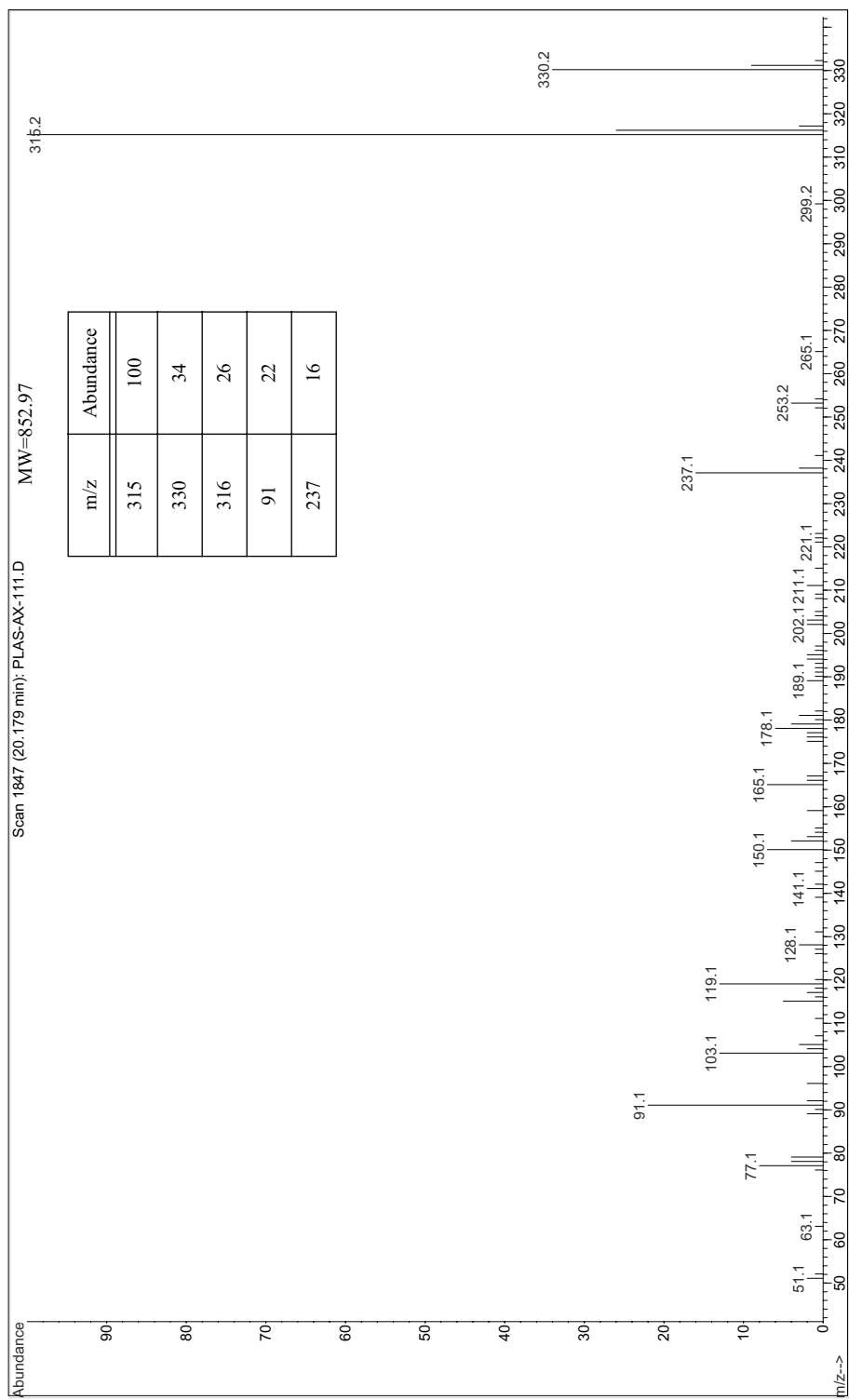
The compound has a large estimated value for K_{oc} (log K_{oc} > 4.3) indicating strong affinity for the organic component of soils and sediments, and the strong binding indicates that it would have low mobility in these media. This compound is not readily biodegradable, but when bound to, or otherwise associated with, soils and sediments it could be expected to be slowly degraded through the agency of biological and abiotic processes operative within landfills.

Point of Release

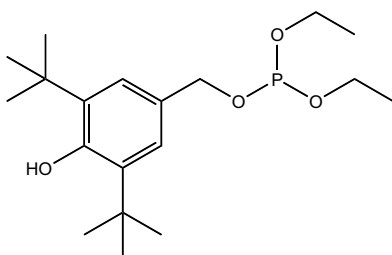
This chemical is not available for sale to the public and will be used as an ingredient in plastics manufacture. The potential for public exposure during transport, reformulation, or disposal is assessed as negligible. The public may make dermal contact with some plastic products and may eat or drink foodstuffs that have been in contact with plastics containing this chemical.

Toxicological DataAcute oral toxicity (LD₅₀): > 5000 mg/kg [Rat]Acute dermal toxicity (LD₅₀): > 2000 mg/kg [Rat]

Mass Spectrum for PLAS-AX-111



For Chromatogram See Appendix A - PLAS-AX-111 - page 480

Diethyl 3,5-Di-tert-butyl-4-hydroxybenzylphosphonate

CAS Number 976-56-7
RTECS Number N/A
Abbreviation Not Identified

Formula C₁₉H₃₃O₄P
Molecular Weight 356.44

Chemical Name

2,6-ditert-butyl-4-(diethoxyphosphorylmethyl)phenol

Synonyms

3,5-di-tert-butyl-4-hydroxybenzylphosphonic acid diethyl ester

Brand Names & Manufacturers

Antioxidant 1222	FuncChem
Irgamod® 295	Ciba (BASF)
Irganox® 4426	Ciba (BASF)

Physical Properties

Appearance	White to light yellow powder					
Melting Point	116-121 °C		Boiling Point N/A			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water 0.01	MeOH 62	EtOH U	Acetone 27	CH₂Cl₂ U	Hexane 20

Application, Regulatory & Environmental Information

Application Used as an antioxidant/stabilizer for polyester polymers (PET) compliant with 21 CFR 177.1630, at levels not to exceed 1100 ppm. Added during the esterification step of the polymerization and is incorporated into the backbone of the PET resin. Used in plastics and synthetic fibers. Protects polyurethanes against oxidative degradation.

Regulatory Information

Approved for food contact under 21 CFR §177.1630.

Environmental Impact

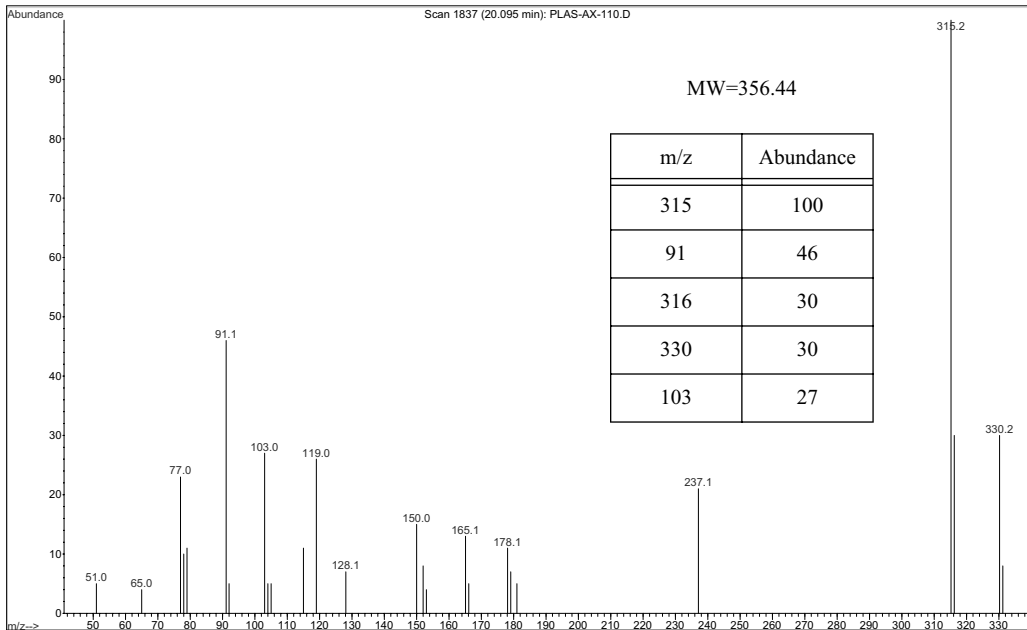
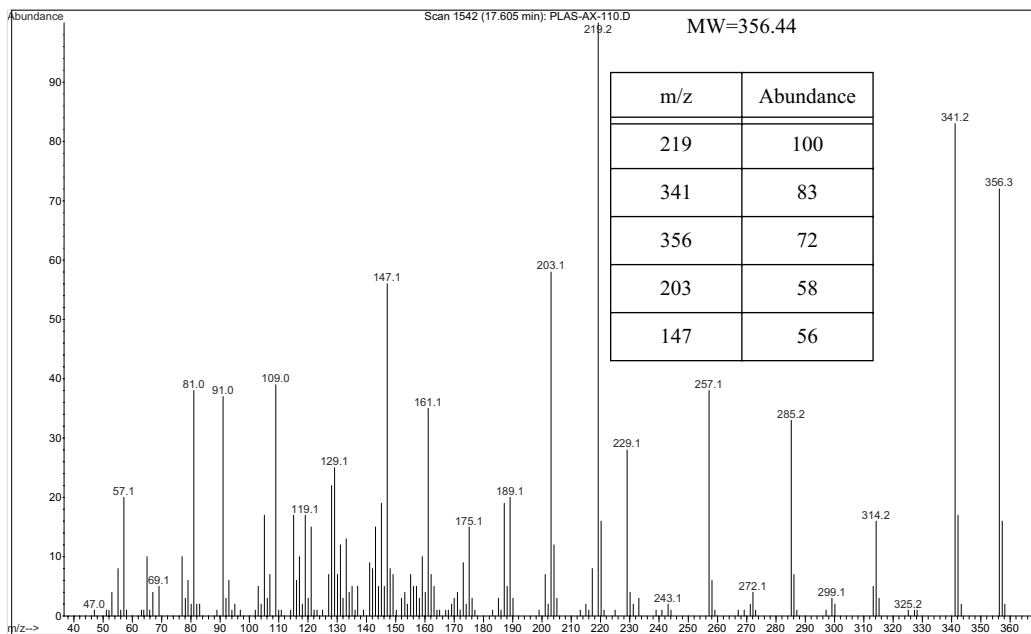
Not expected to have adverse environmental effects because only small quantities, if any, of substances will be introduced into the environment as a result of the use and disposal of PET resin. In addition, any substance released from the disposal of a PET resin that contains this product is not expected to be different than from an existing PET resin.

Point of Release

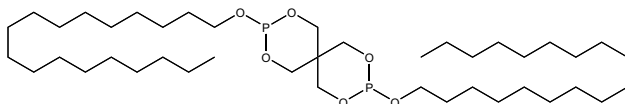
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): >5000 mg/kg [Mouse]

Mass Spectra for Diethyl 3,5-Di-*tert*-butyl-4-hydroxybenzylphosphonate - PLAS-AX-110

For Chromatogram See Appendix A - PLAS-AX-110 - page 481

O,O'-Diocetadecylpentaerythritol bis(phosphite)**CAS Number** 3806-34-6**RTECS Number** N/A**Abbreviation** DPEDP**Formula** C₄₁H₈₂O₆P₂**Molecular Weight** 733.03**Chemical Name**

O,O'-diocetadecylpentaerythritol bis(phosphite)

Synonyms

O,O'-diocetadecylpentaerythritol bis(phosphite); distearyl pentaerythritol diphosphite

Brand Names & Manufacturers

Cristol-DPEDP
 Doverphos® S-680
 Songnox® 6180
 Weston 618F

Krishna
 Dover Chemical Corporation
 Songwon
 Chemtura

Physical Properties**Appearance** Flakes**Melting Point** 44-47 °C**Boiling Point** 705 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	U	0.3	U	25

Application, Regulatory & Environmental Information

Application Used as a secondary antioxidant in powder and coil coating formulations. Prevents discoloration and loss of physical properties. Also used as an antioxidant in PE, PP, PS, ABS, PVC, and polybutadiene.

Regulatory Information

Approved for food contact FDA 21CFR §176.170, §178.2010, and §177.1520

Environmental Impact

Acute/prolonged toxicity to fish: LC50 = 2.94E-10 mg/L

LC50 = 7.76E-10 mg/L [Crustacea]

EC50 = 1.03E-09 mg/L [Algae]

Not readily biodegradable.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

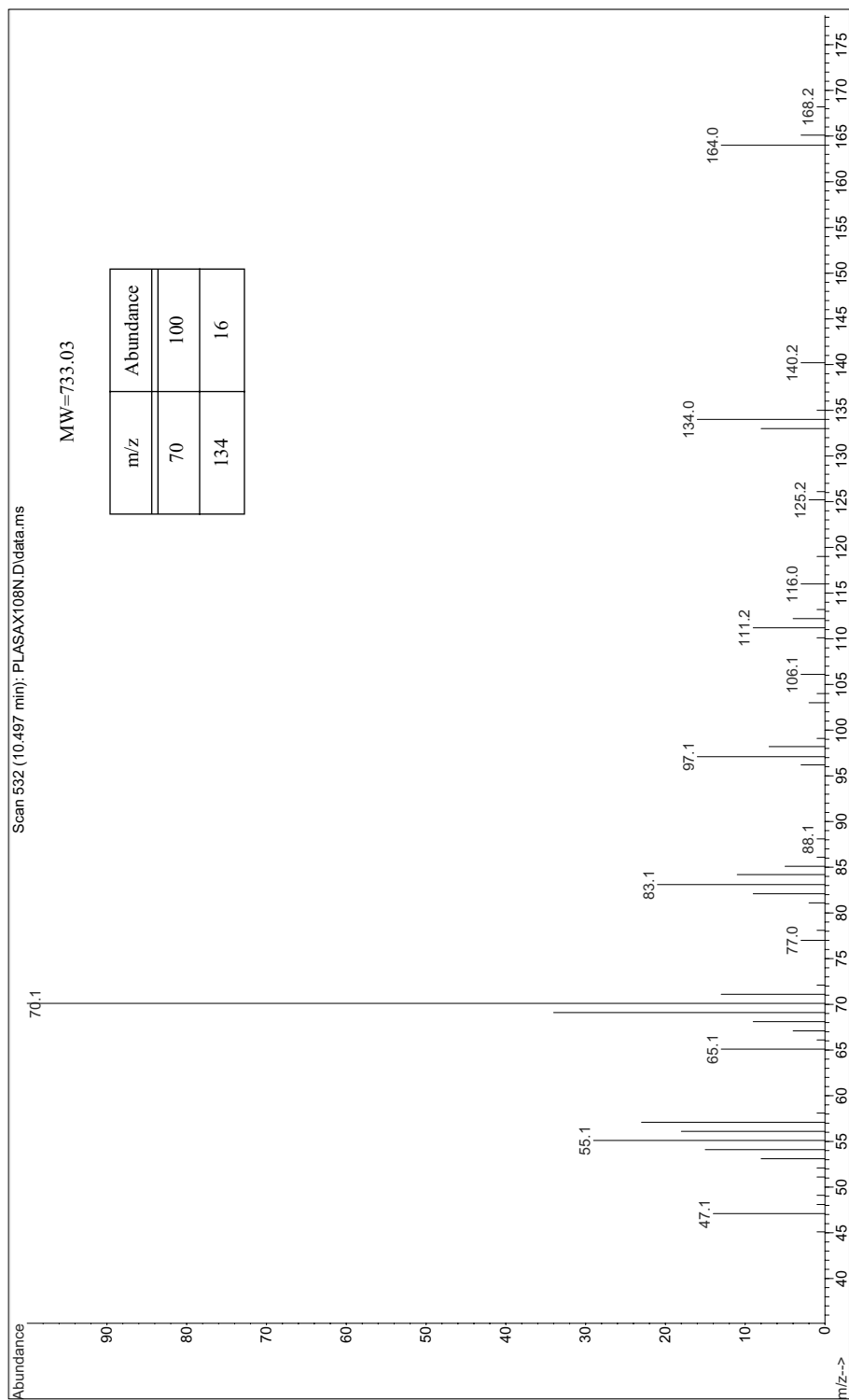
Toxicological Data

Oral LD50: >1000 mg/kg [Rat]

Dermal LD50: >2000 mg/kg [Rabbit]

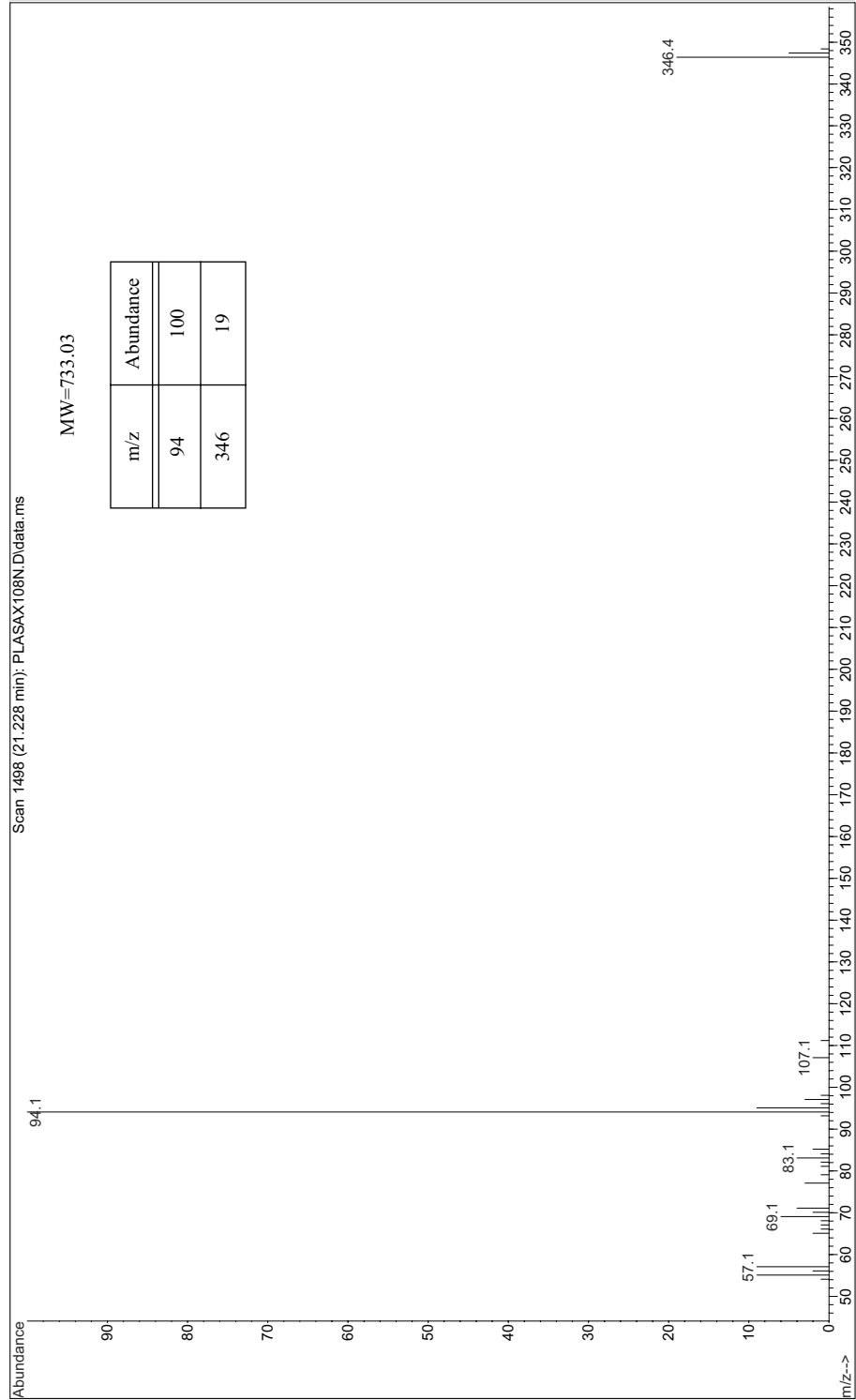
NOAEL >3000 ppm

Mass Spectrum for O,O'-Diocetadecylpentaerythritol bis(phosphite) - PLAS-AX-108



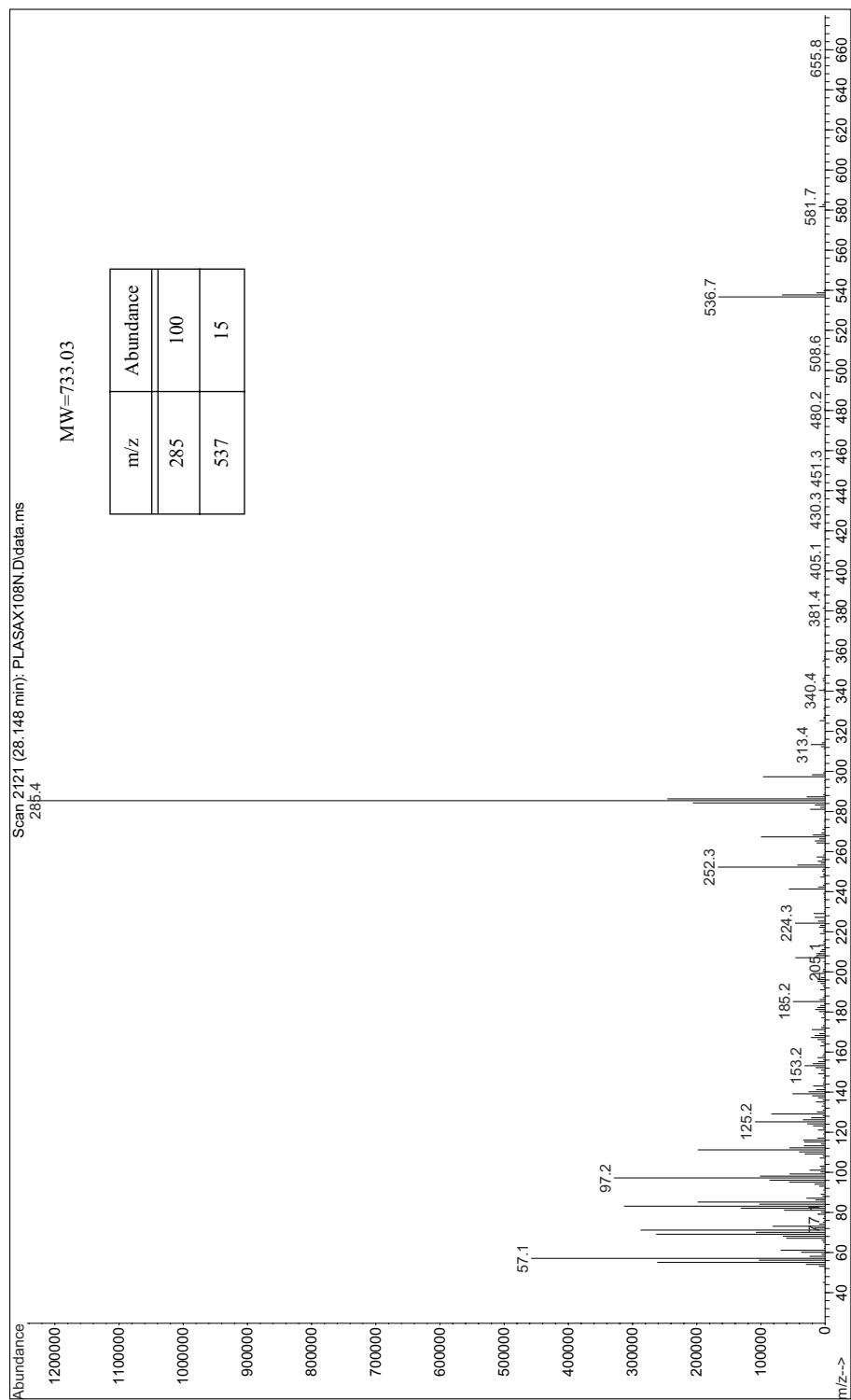
For Chromatogram See Appendix A - PLAS-AX-108 - page 482

Mass Spectrum for O,O'-Diocetadecylpentaerythritol bis(phosphite) - PLAS-AX-108



For Chromatogram See Appendix A - PLAS-AX-108 - page 482

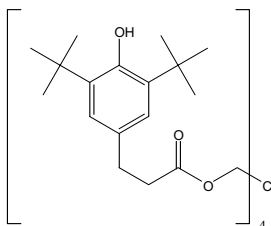
Mass Spectrum for O,O'-Diocetadecylpentaerythritol bis(phosphite) - PLAS-AX-108



For Chromatogram See Appendix A - PLAS-AX-108 - page 482

Ethanox® 310

Albemarle Corporation

**CAS Number** 6683-19-8**RTECS Number** DA8340000**Abbreviation** PE**Formula** C₇₃H₁₀₈O₁₇**Molecular Weight** 1177.65**Chemical Name**pentaerythritol tetrakis (3-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionate**Synonyms**

2,2-bis{3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy}-1,3-propanediyl ester

Brand Names & Manufacturers

Anox® 20	Chemtura Corporation
Ultranox® 210	Chemtura Corporation
Irganox® 1010	Ciba Specialty Chemicals
Cyanox® 2110 (EF)	Cytec Technology Corp.

Physical Properties

Appearance	White crystalline powder					
Melting Point	110-125 °C			Boiling Point	Not available	
Stability	Stable at normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH 0.9	EtOH 1.5	Acetone 47	CH₂Cl₂ 63	Hexane 0.3

Application, Regulatory & Environmental Information**Application**

Used as an antioxidant and thermostabilizer for polypropylene, polyethylene, impact resistant polystyrene, poly-4-methyl-pentene. Can be used as a stabilizer for natural and synthetic rubber, polyvinyl chloride, and copolymers of acrylonitrile with butadiene and styrene, polyacetals, alkyde resins, polyamides, and polyesters.

Regulatory Information

FDA approved for use in indirect food contact applications.

British Standard — Listed as an antioxidant for polyethylene and polypropylene compositions used in contact with food-stuffs or water intended for human consumption (max permitted in final compound 0.5%).

Environmental Impact

Experimental data shows that this category of chemicals is not readily biodegradable. This class of compounds photodegrades rapidly. In the environment, occurrence would be partitioned primarily to soil and sediments rather than air or water.

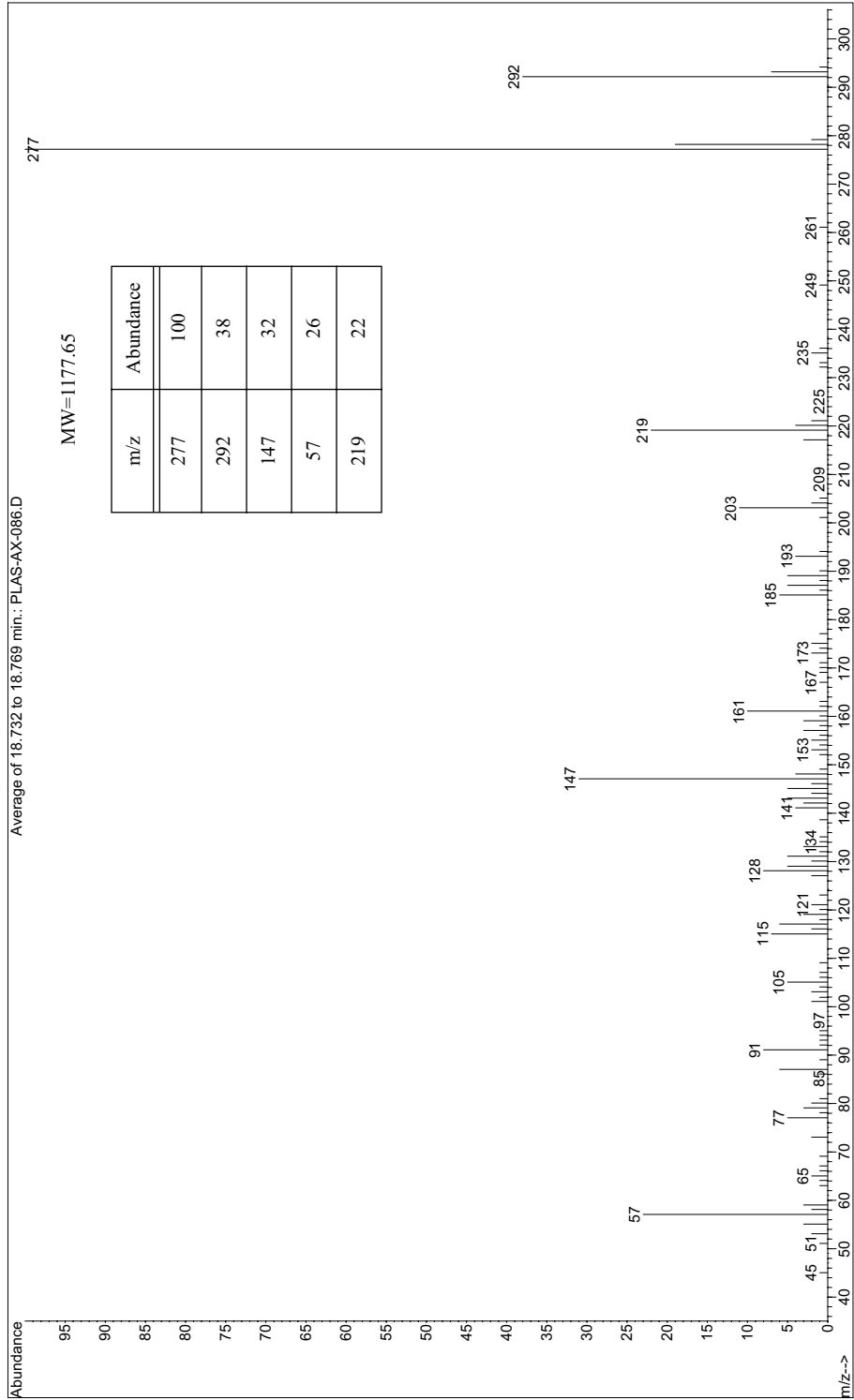
Point of Release

Migration is greater from polypropylene than from high-density polyethylene. Little migration is found to aqueous media. Migration is highest into *n*-heptane, ethanol, and corn oil.

Toxicological Data

Toxicity of this compound is considered low. LD50 was not quantitated, rats tolerated administration of 5.0 g/kg body weight and mice tolerated up to 10 mg/kg body weight.

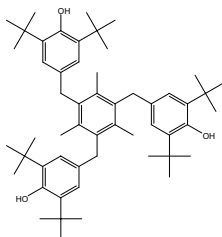
Mass Spectrum for *Ethanox*[®] 310 - PLAS-AX-086



For Chromatogram See Appendix A - PLAS-AX-086 - page 483

Ethanox[®] 330

Albemarle Corporation

**CAS Number** 1709-70-2**RTECS Number** DC3750000**Abbreviation** Not Identified**Formula** C₅₄H₇₈O₃**Molecular Weight** 775.32**Chemical Name**

1,3,5-trimethyl-2,4,6-tris(3,5-di-tert-butyl-4-hydroxybenzyl) benzene

Synonyms

4,4',4''-((2,4,6-trimethyl-1,3,5-benzenetriyl)tris(methylene))tris (2,6-bis(1,1-dimethylethyl)phenol); methylene bis ethyl butyl phenol; 2,4,6-Tri-(3',5'-di-tert-butyl-4'-hydroxybenzyl)mestitylene

Brand Names & Manufacturers

Anox [®] 330	Chemtura Corporation
Antioxidant 330	Akrochem Corporation
Ionox [®] 330	Shell Oil Company
Irganox [®] 330	Ciba Specialty Chemicals

Physical Properties

Appearance	White crystalline powder					
Melting Point	240-245 °C			Boiling Point	822 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH 0.2	EtOH U	Acetone 23.0	CH₂Cl₂ 47.0	Hexane 1.7

Application, Regulatory & Environmental Information**Application**

Ethanox[®] 330 is a phenolic stabilizer for manufacturing synthetic rubber, mineral oils, and oils in some food products; providing protection from light and heat aging, and for light and colored rubbers. May also be used as a thermo stabilizer for polyethylene and polypropylene fiber. High molecular weight phenolic antioxidants are commonly used in a wide variety of applications, including elastomers, hot melt adhesives, tackifiers, and engineering blends.

Regulatory Information

Ethanox[®] 330 is allowed by the FDA in all polymers for food contact applications subject to the limitations provided in 21CFR178.2010.

Environmental Impact

This compound has a calculated partition coefficient (log Pow) of > 6. Based on this and its other physical-chemical properties, the substance in the environment is likely to bind to the soil and sediment where it is expected to be immobile and have limited bioavailability. The material is not readily biodegradable.

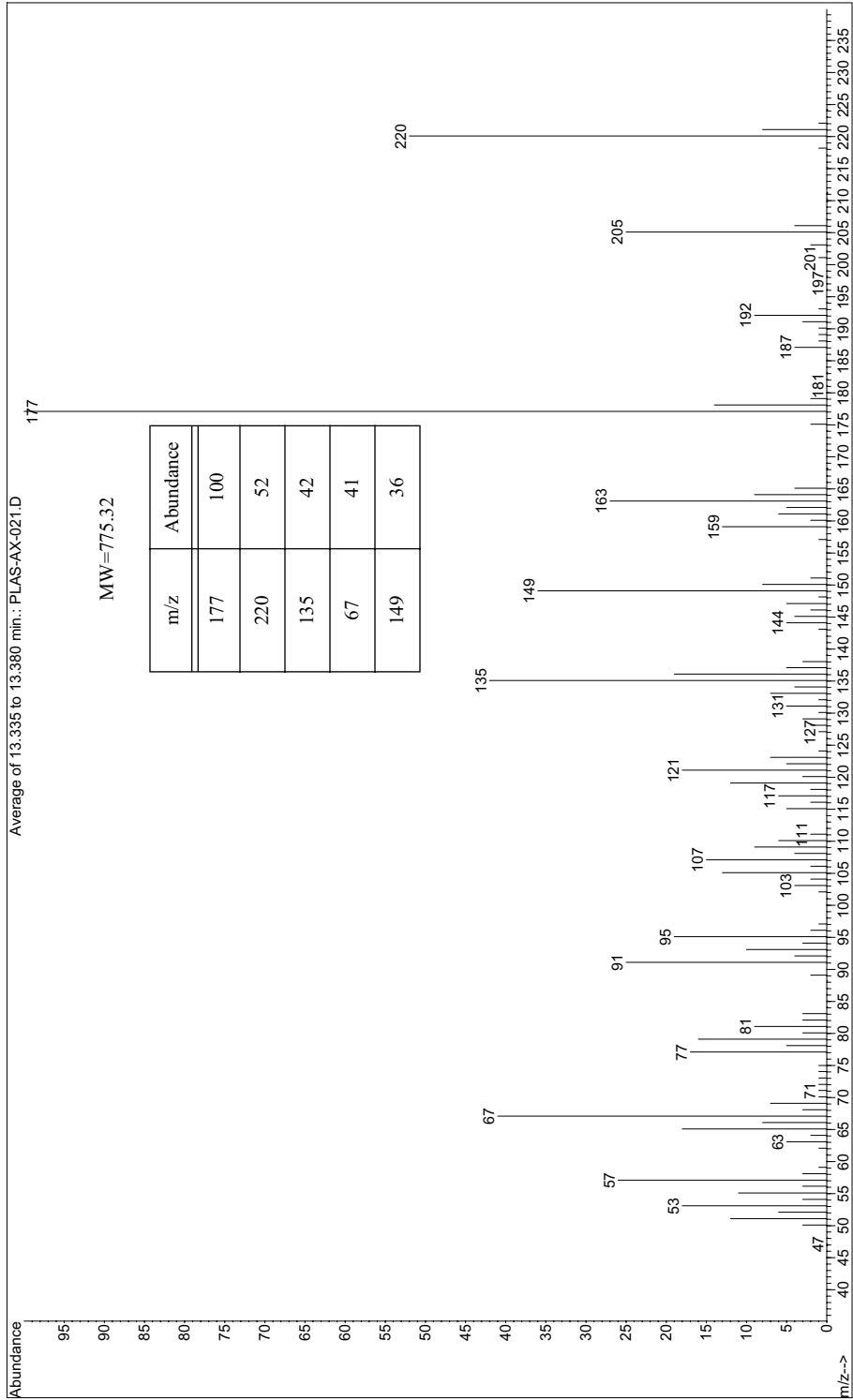
Point of Release

When Ethanox[®] 330 is incorporated in the polymer matrix, it is relatively immobile and release-exposure to humans or the environment is considered minimal.

Toxicological Data

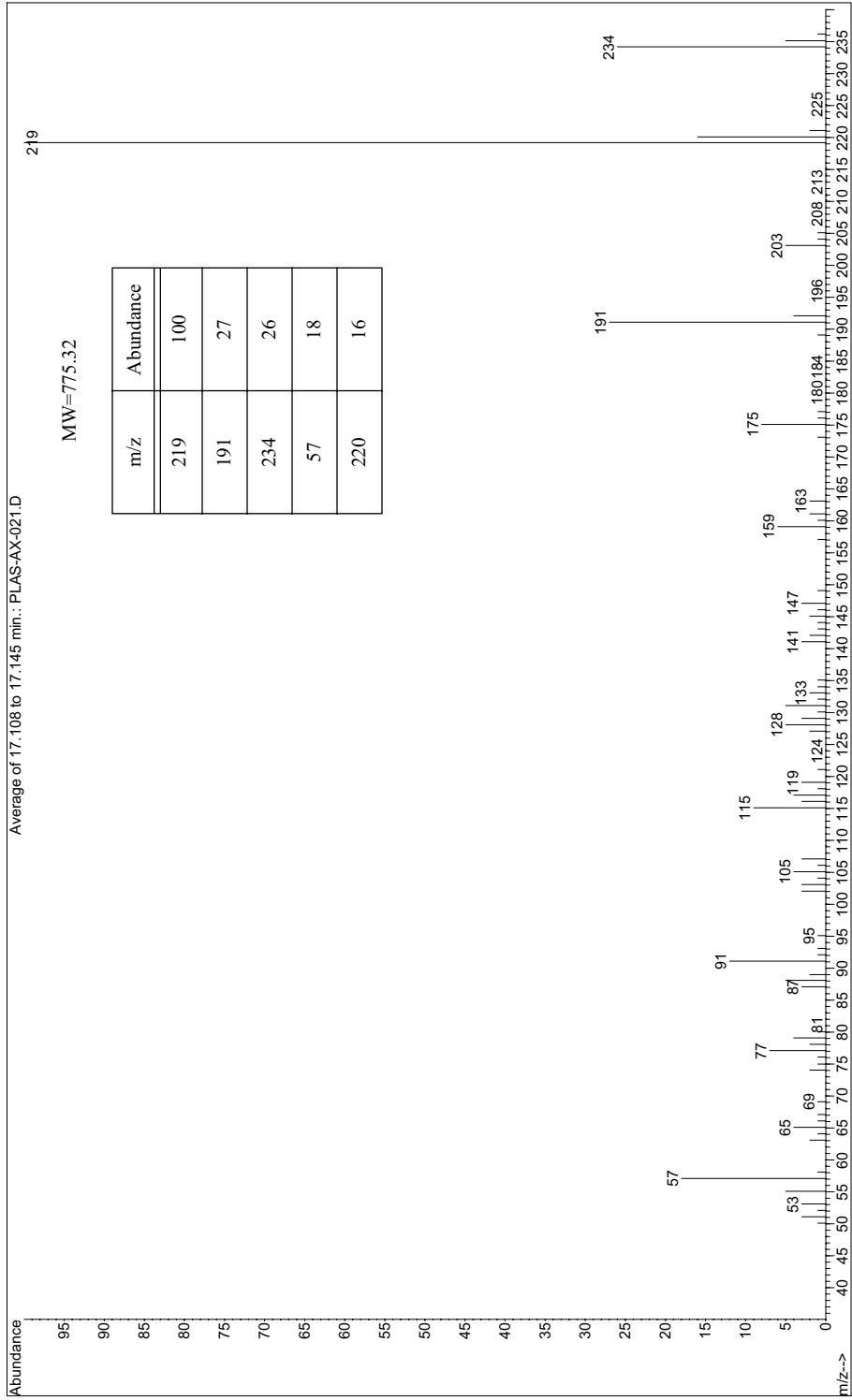
RTECS CLASS OF COMPOUND: Reproductive effector. Acute oral toxicity (LD50): 1100 mg/kg [Rat]. Lowest published toxic oral dose (TDLo): 5000 mg/kg [Rat].

Mass Spectrum for *Ethanox*[®] 330 - PLAS-AX-021



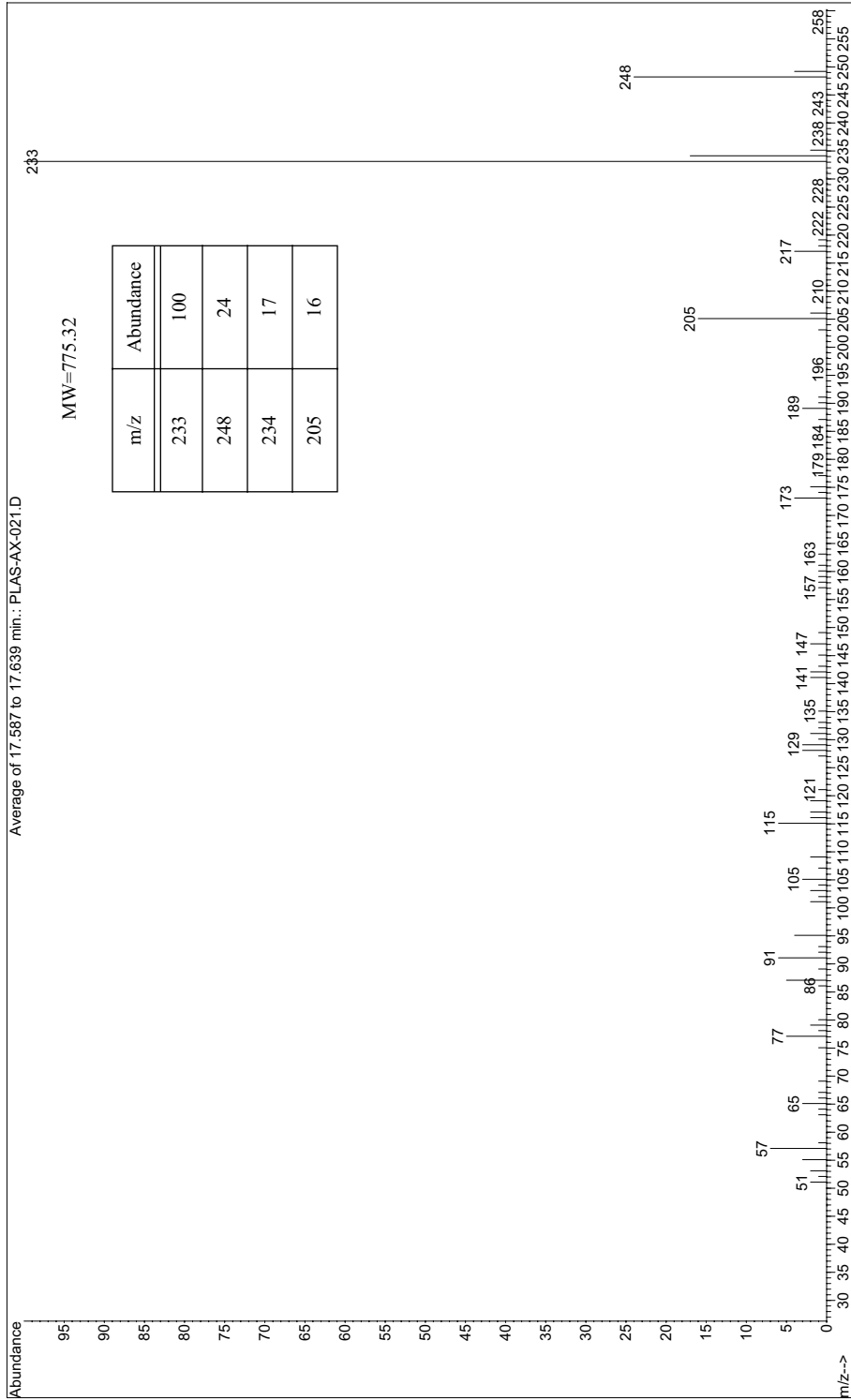
For Chromatogram See Appendix A - PLAS-AX-021 - page 484

Mass Spectrum for *Ethanox*[®] 330 - PLAS-AX-021



For Chromatogram See Appendix A - PLAS-AX-021 - page 484

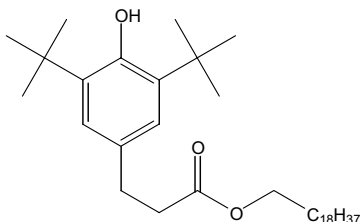
Mass Spectrum for *Ethanox*[®] 330 - PLAS-AX-021



For Chromatogram See Appendix A - PLAS-AX-021 - page 484

Ethanox[®] 376

Albemarle Corporation

**CAS Number** 2082-79-3**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₃₅H₆₂O₃**Molecular Weight** 530.87**Chemical Name**

3,5-di-tert-butyl-4-hydroxyhydrocinnamic acid, octadecyl ester

Synonyms

octadecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate; stearyl 3-(4-hydroxy-3,5-di-tert-butyl-4-hydroxyphenyl)propionate; 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid

Brand Names & ManufacturersAnox[®] PP 18

Chemtura Corporation

Antioxidant 1076

Akrochem Corporation

Irganox[®] 1076

Ciba Specialty Chemicals

Naugard[®] 76

Chemtura Corporation

Physical Properties**Appearance** White or yellowish crystalline powder**Melting Point** 50-55 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.6	1.5	19	U	32

Application, Regulatory & Environmental Information

Application Ethanox[®] 376 is a stabilizer that provides heat stability by preventing thermo-oxidative degradation during processing and service life. It provides compatibility with resins and extraction resistance. It can be applied in polyolefins, such as polyethylene, polypropylene, polybutene-1, and other polymers such as engineering plastics, styrenes, polyurethanes, saturated and unsaturated elastomers, styrenics, rubber modified styrenics, segmented block copolymers, and PVC.

Regulatory Information

FDA approved for use in indirect food contact applications.

Environmental Impact

This product is of low toxicity to aquatic organisms.

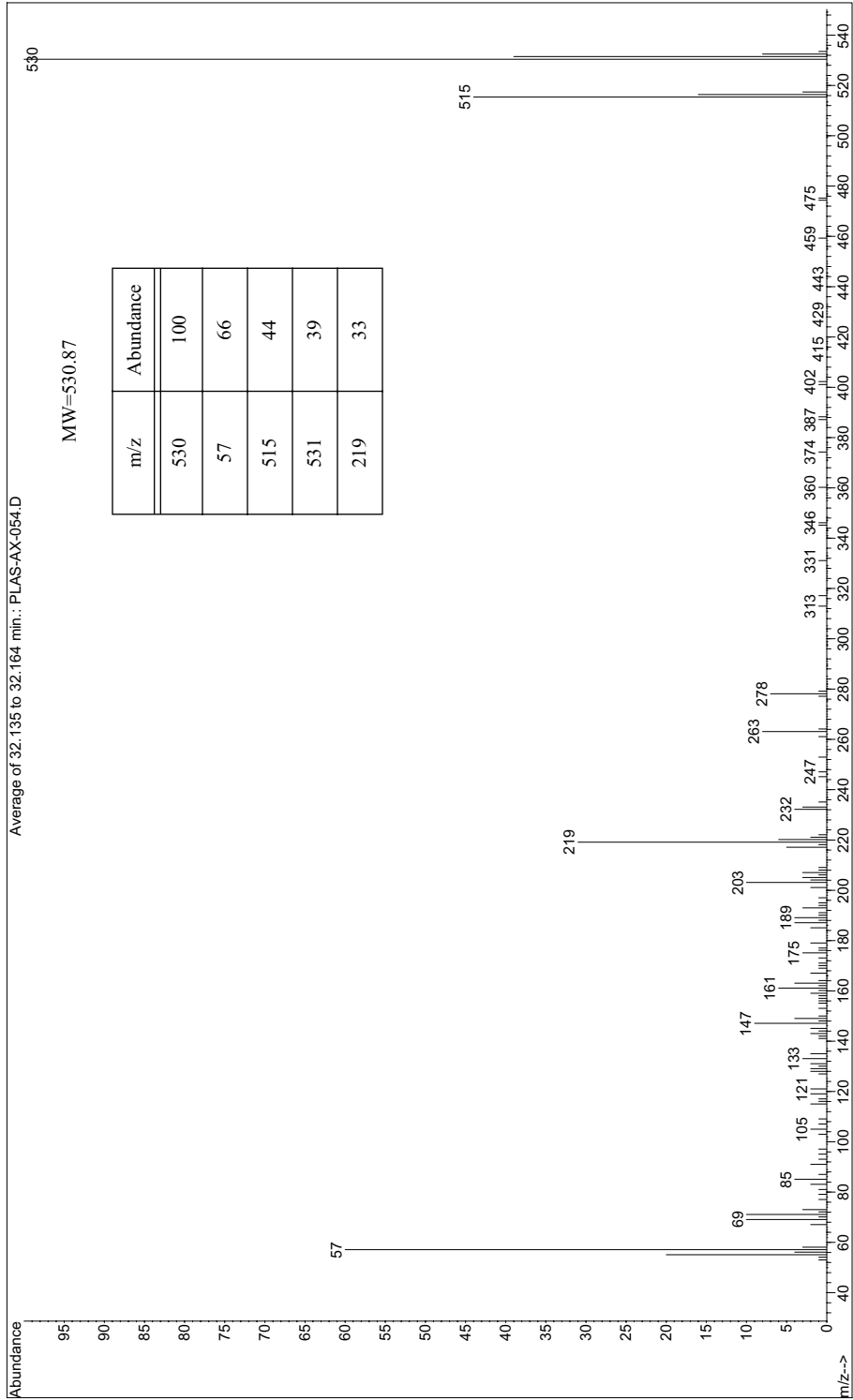
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

This product presents little or no immediate hazard to people if spilled or released. Acute oral toxicity (LD50) > 6000 mg/kg [Hamster], >10,000 mg/kg [Rat]; acute dermal toxicity (LD50): [Rabbit] >2000 mg/kg; acute inhalation toxicity: (LC50) > 1.8 mg/l [Rat] air for a 4-hour dust exposure with approximately 90% of particles > 7μ diameter. There were no mortalities at this concentration.

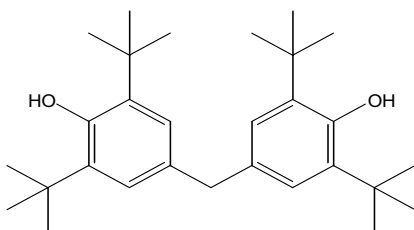
Mass Spectrum for *Ethanox*[®] 376 - PLAS-AX-054



For Chromatogram See Appendix A - PLAS-AX-054 - page 485

Ethanox[®] 702

Albemarle Corporation

**CAS Number** 118-82-1**RTECS Number** SL9650000**Abbreviation** TBMD**Formula** C₂₉H₄₄O₂**Molecular Weight** 424.66**Chemical Name**

4,4'-methylenebis(2,6-di-tert-butylphenol)

Synonyms

di(4-hydroxy-3,5-di-tert-butylphenyl)methane

Brand Names & ManufacturersIono[®] 220

Degussa

Physical Properties**Appearance** Light-yellow fine crystals**Melting Point** 155 °C**Boiling Point** 289 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 1-10	EtOH 1-10	Acetone U	CH₂Cl₂ U	Hexane 1-10
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Application **Application, Regulatory & Environmental Information**

This material may be used in natural and synthetic elastomers, polyolefin plastics, resins, adhesives, petroleum oil, and waxes.

Regulatory Information

This material is approved by the FDA, as specified in 21CFR in the following applications: adhesives and polymers in food contact in the following polymers: petroleum hydrocarbon resins, polyethylene, and polybutadiene.

Environmental Impact

Products of degradation may produce persistent bioaccumulative toxins.

96H (LC50): ~ 1000 mg/L [Fathead minnow], 48 hour (LC50): ~ 1000 mg/L [Daphnia Magna].

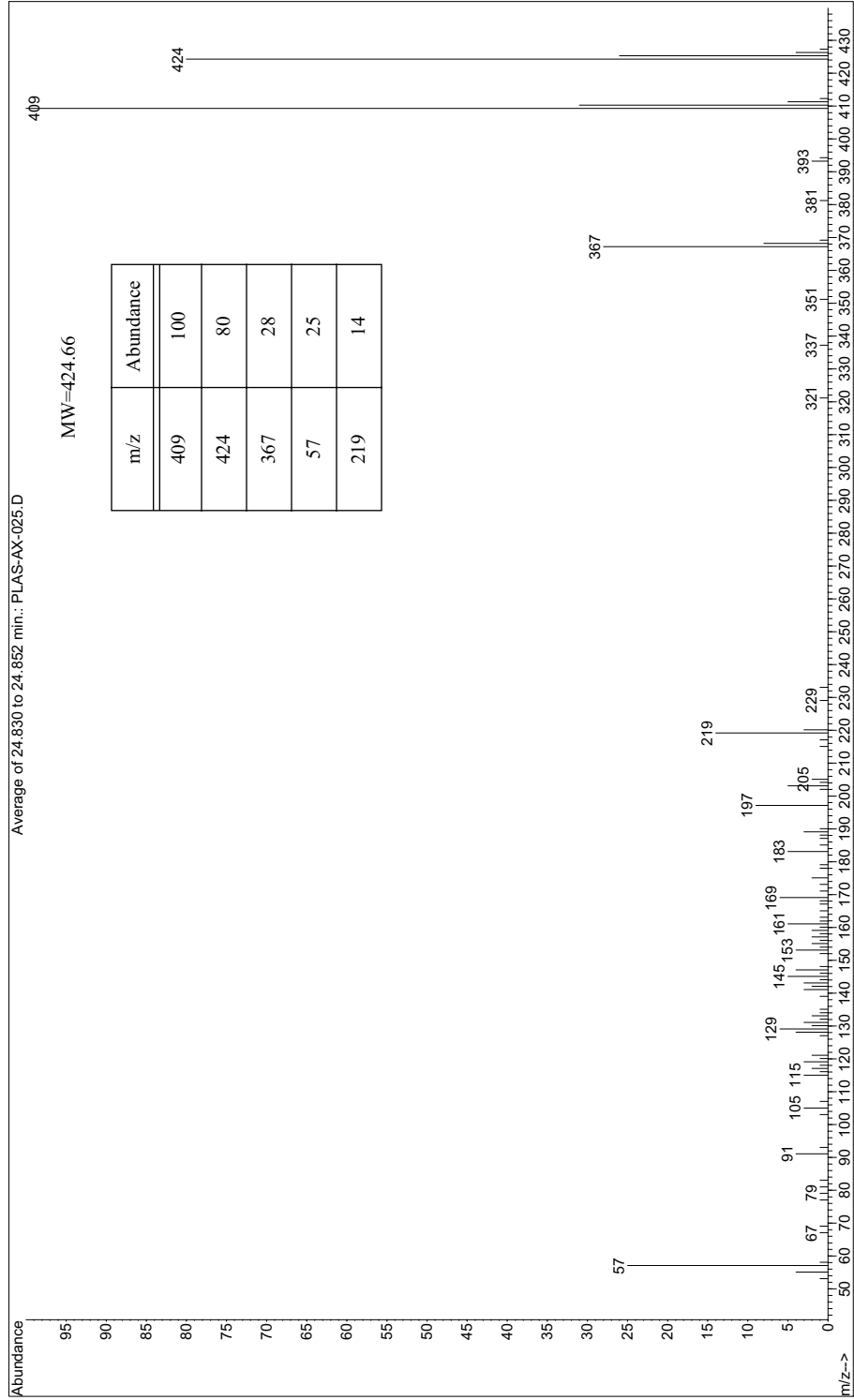
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral toxicity (LD50): >24000 mg/kg [Rat]; acute dermal toxicity (LD50): >2000 mg/kg [Rat].

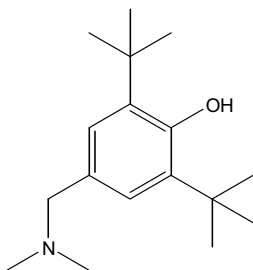
Mass Spectrum for *Ethanox*[®] 702 - PLAS-AX-025



For Chromatogram See Appendix A - PLAS-AX-025 - page 486

Ethanox[®] 703

Albemarle Corporation

**CAS Number** 88-27-7**RTECS Number** GO7887000**Abbreviation** Not Identified**Formula** C₁₇H₂₉NO**Molecular Weight** 263.42**Chemical Name**

2,6-di-tert-butyl-N,N-dimethylamino-p-cresol

Synonyms

4-((dimethylamino)methyl)-2,6-bis(1,1-dimethylethyl)phenol

Brand Names & Manufacturers

Ethanox 703

Albemarle Corporation

Physical Properties**Appearance** Light-yellow powder**Melting Point** 93-94 °C**Boiling Point** 172 °C (30 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 1-10	EtOH 10-40	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Ethanox[®] 703 antioxidant is used as an oxidation inhibitor in natural and synthetic elastomers, polyolefin plastics, resins, adhesives, petroleum oil, and waxes. Applications include steam turbine oils, hydraulic fluids, transformer oils, industrial gear oils, and greases.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

This material is not biodegradable, but low log Kow value indicates that it will not bioaccumulate. Degradation byproducts may produce persistent bioaccumulative toxins.

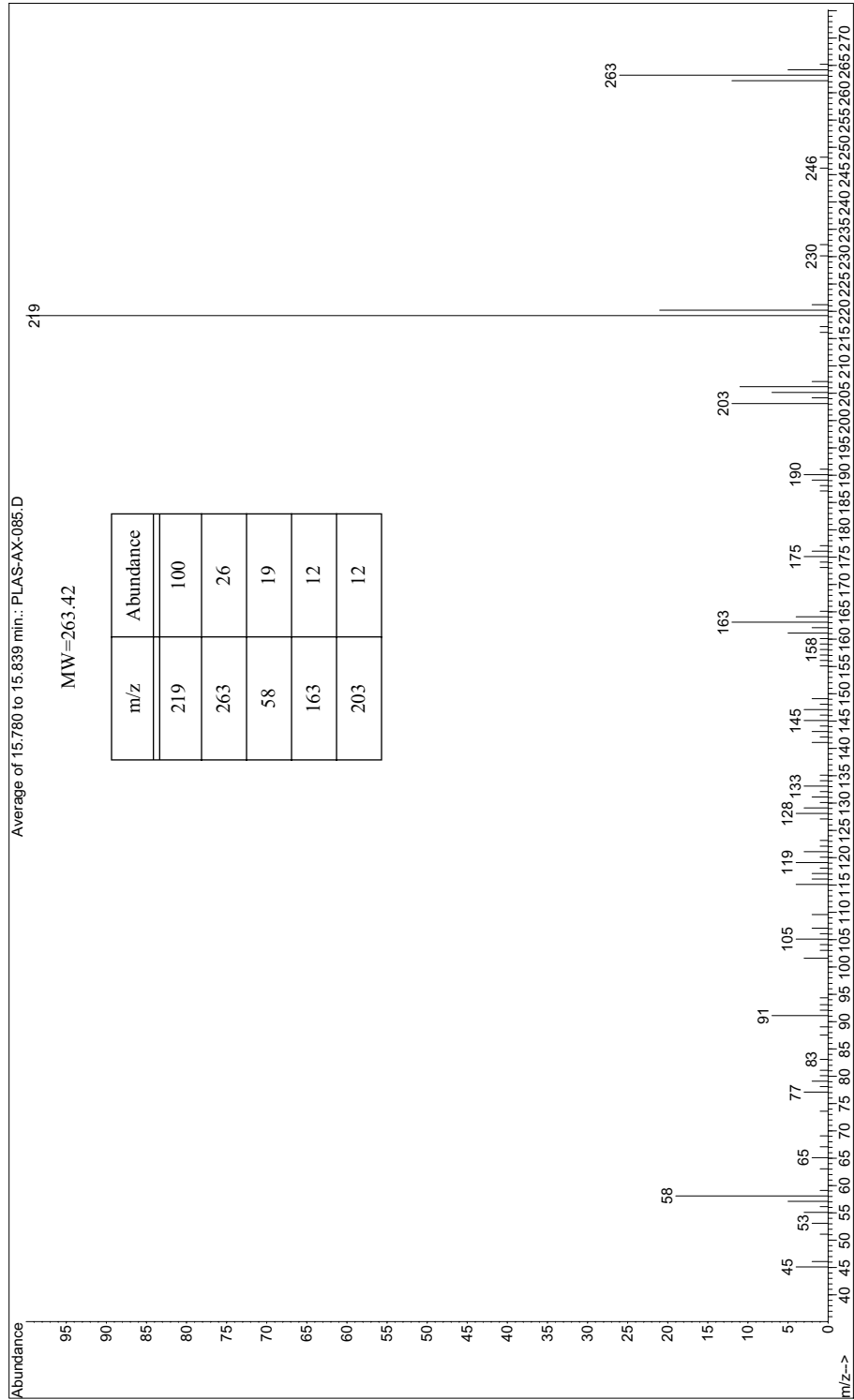
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral toxicity (LD50): 1030 mg/kg [Rat]; dermal (LD50): 4000 mg/kg [Rabbit]. This material is a severe, but reversible, eye irritant.

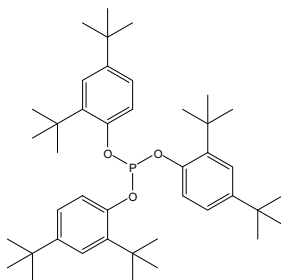
Mass Spectrum for *Ethanox*[®] 703 - PLAS-AX-085



For Chromatogram See Appendix A - PLAS-AX-085 - page 487

Ethaphos® 368

Albemarle Corporation

**CAS Number** 31570-04-4**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₄₂H₆₃O₃P**Molecular Weight** 646.92**Chemical Name**

tris(2,4-di-tert-butylphenyl) phosphite

Synonyms

2,4-bis(1,1-dimethylethyl)phenol, phosphite (3:1)

Brand Names & Manufacturers

Alkanox® 240

Chemtura Corporation

Irgafos® 168

Ciba Specialty Chemicals

Naugard® 524

Chemtura Corporation

Ultranox® 668

Chemtura Corporation

Physical Properties**Appearance** White crystalline powder**Melting Point** 183-187 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	<0.01	0.1	1	36	11

Application, Regulatory & Environmental Information**Application** Phosphite processing stabilizer for polypropylene, polyethylene, and adhesives.**Regulatory Information**

FDA approved for indirect food contact applications.

Environmental Impact

Potential for slight bioaccumulation, not readily biodegradable log Pow >6 (calculated). (LC50 96 hour): > 100 mg/L [Fish], no effects at the highest tested concentration. The tested concentration is well above its water solubility. (EC50 24 hour): 510 mg/L [Daphnia].

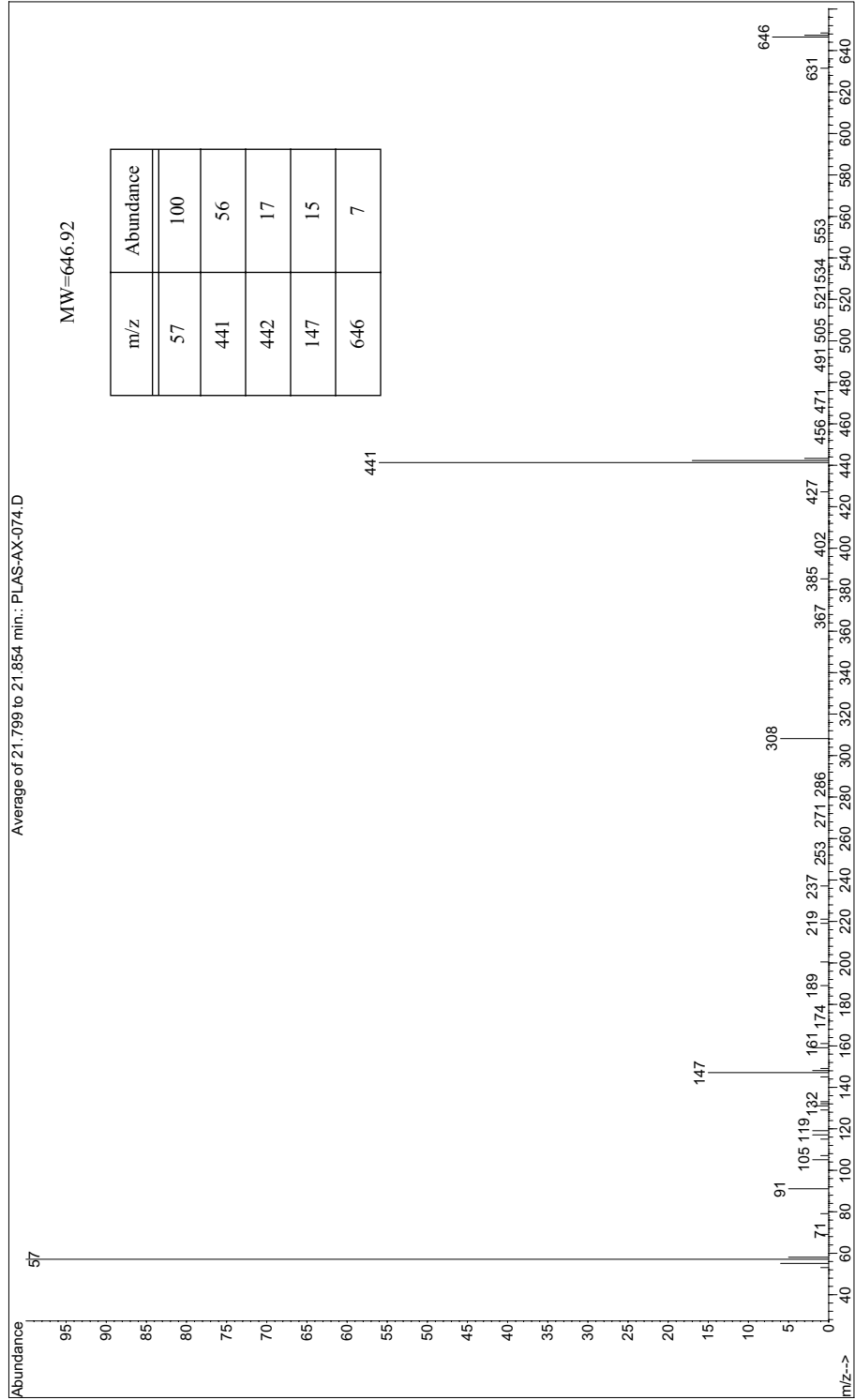
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

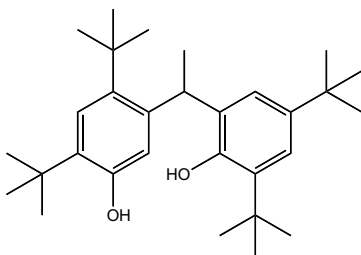
Toxicological Data

Not regarded as a health or environmental hazard under current legislation. Acute oral toxicity (LD50): > 2000 mg/kg [Rat]; acute skin toxicity (LD50): > 2000 mg/kg [Rat].

Mass Spectrum for Ethaphos® 368 - PLAS-AX-074



For Chromatogram See Appendix A - PLAS-AX-074 - page 489

2,2'-Ethylidene-bis(4,6-di-tert-butylphenol)**CAS Number** 35958-30-6**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₃₀H₄₆O₂**Molecular Weight** 438.69**Chemical Name**

2,4-ditert-butyl-6-[1-(3,5-ditert-butyl-2-hydroxyphenyl)ethyl]phenol

Synonyms

2,2'-ethylidenebis[4,6-bis(1,1-dimethylethyl)-phenol]

Brand Names & ManufacturersEthanox[®] 308

Albemarle

Irganox[®] 129

Ciba (BASF)

Songnox[®] 1290

Songwon

Vanox[®] 1290

RT Vanderbilt

Physical Properties**Appearance** White to off-white pellets or powder**Melting Point** 162-164 °C**Boiling Point** 465 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.03	MeOH U	EtOH U	Acetone >100	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Used in adhesives. Offers protection against thermo-oxidative degradation during processing, storage, and end-use. Reacts synergistically with thiosynergists to enhance thermal aging properties of polypropylene. Provides stabilization in crystalline and high impact polystyrene, ABS terpolymer, PVC, polyamides, polyurethanes, elastomers, rubbers such as EPDM, SBS and rubber blends with polyolefins, and natural and synthetic tackifier resins.

Regulatory Information

FDA 21CFR §175.105 (Indirect food additives - adhesives), §178.2010.

Environmental Impact

Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

Point of Release

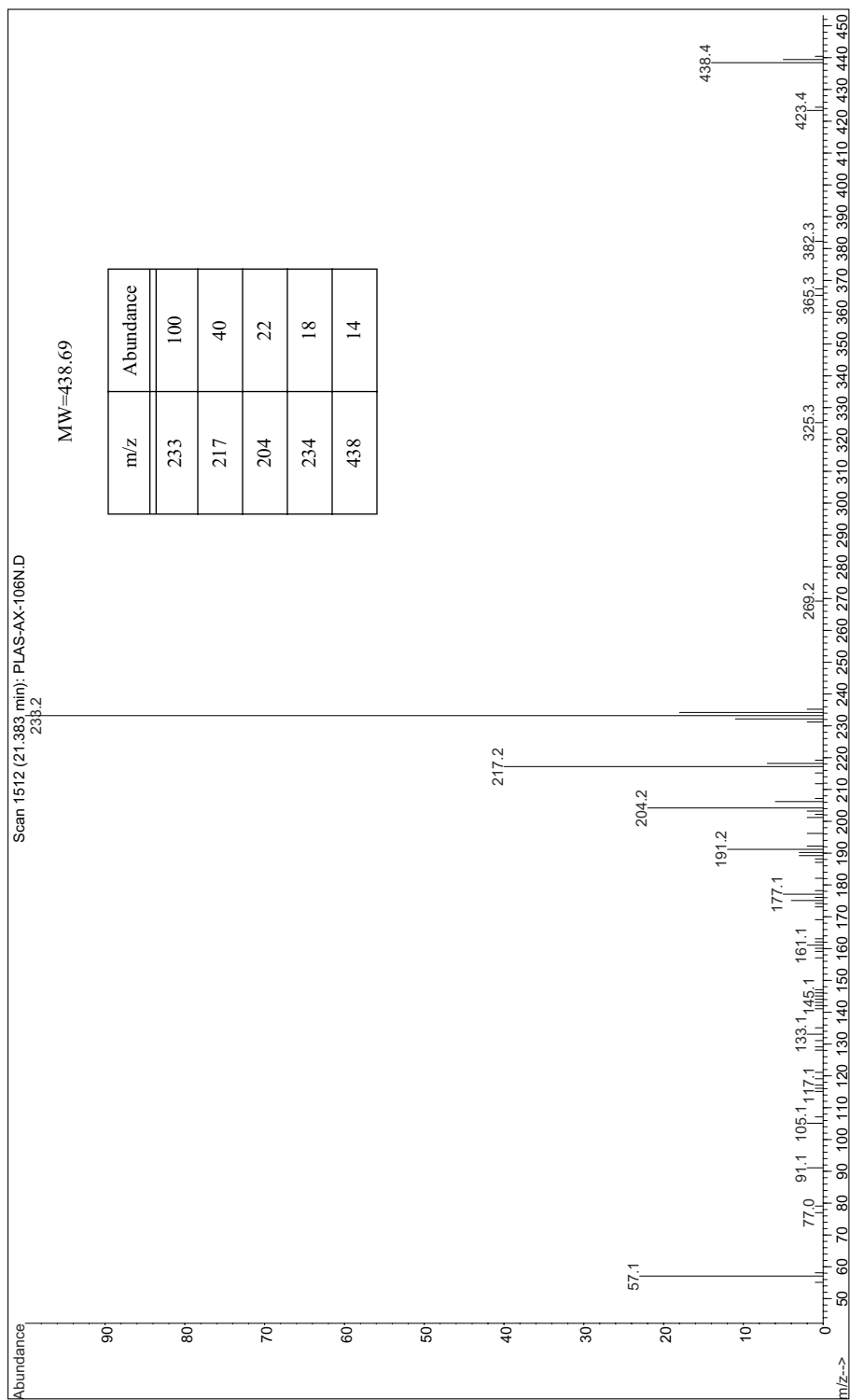
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

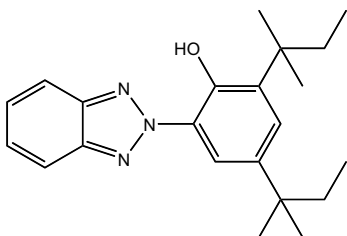
Oral LD50: >1000 mg/kg [Rat]

Skin LD50: >2000 mg/kg [Rabbit]

Mass Spectrum for 2,2'-Ethylidene-bis(4,6-di-tert-butylphenol) - PLAS-AX-106



For Chromatogram See Appendix A - PLAS-AX-106 - page 488

2-(2'-Hydroxy-3',5'-di-tert-amylphenyl) benzotriazole**CAS Number** 25973-55-1**RTECS Number** MFCD00142737**Abbreviation** Not Identified**Formula** C₂₂H₂₉N₃O**Molecular Weight** 351.49**Chemical Name**

2-(benzotriazol-2-yl)-4,6-bis(2-methylbutan-2-yl)phenol

Synonyms

2-(3,5-di-tert-pentyl-2-hydroxyphenyl) benzotriazole

Brand Names & Manufacturers

BLS® 1328

Mayzo

Eversorb® 74

Everlight Chemical

Lowilite® 28

Chemtura

Tinuvin® 328

Ciba

Physical Properties**Appearance** Slight yellow powder**Melting Point** 80-88 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.4	U	6	56	16

Application, Regulatory & Environmental Information**Application**

Suitable for light stabilizing in coatings, propylene, polyurethane, PVC, unsaturated polyester, polyacrylate, polycarbonate, rigid and flexible polyvinyl chloride, ABS, epoxy, acrylic, and polystyrene.

Regulatory Information

Not intended for use in applications that come in contact with food or in products that may come in contact with mucous membranes or abraded skin or be implanted into the body. May be used in adhesives complying with Title 21, CFR §175.105.

Environmental Impact

LC50 in zebra fish (96 hour): >100mg/L

EC50 (algae): > 10 ppm

Not readily biodegradable.

Point of Release

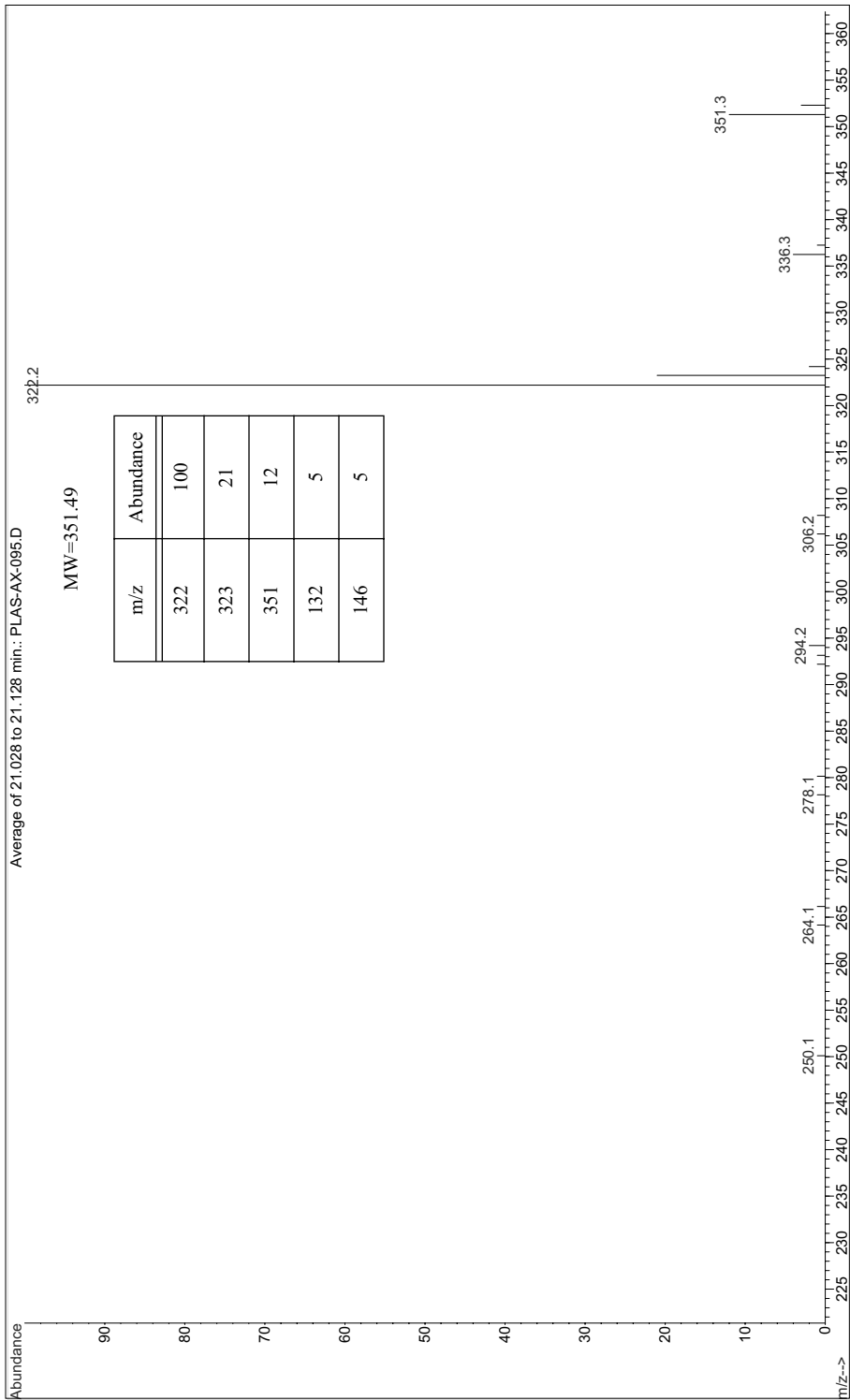
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): 5000 mg/kg [Rat]

No effects on reproductive organs in repeat dose testing.

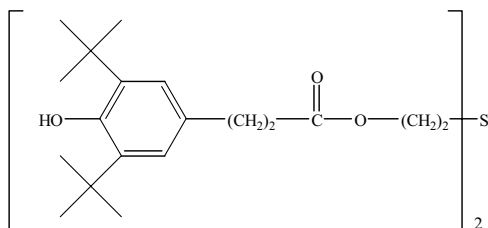
Mass Spectrum for 2-(2'-Hydroxy-3',5'-di-tert-amylphenyl) benzotriazole - PLAS-AX-095



For Chromatogram See Appendix A - PLAS-AX-095 - page 490

Irganox® 1035

Ciba Specialty Chemicals

**CAS Number** 41484-35-9**RTECS Number** DA8342500**Abbreviation** Not Identified**Formula** C₃₈H₅₈O₆S**Molecular Weight** 642.93**Chemical Name**

thiodiethylene bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate)

Synonyms

3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid thiodi-2,1-ethanediyl ester; 2,2'-thio-bis{ethyl-B-(3,5-ditertbutyl-4-hydroxyphenyl)}-propionate

Brand Names & Manufacturers

Anox® 70

Naugard® EL-50

BNX® 1035

Chemtura Corporation

Chemtura Corporation

Mayzo, Inc.

Physical Properties**Appearance** White to off-white crystalline powder**Melting Point** 63-78 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	5	U	56	U	5

Application, Regulatory & Environmental Information

Application Non-discoloring, sulfur containing phenolic antioxidant and stabilizer that provides long-term heat stability by preventing thermo-oxidative degradation. Used for the process stabilization of polyethylene wire and cable resins; for polyethylene during extruder compounding. Can also be applied in styrenic polymers, polypropylene, elastomers such as EPDM and SBR, and for carboxylated SBR latex, polybutadiene rubber, and polyisopropene rubber.

Regulatory Information

This compound has been approved by the FDA as an indirect food additive for use "in polymers, resins or adhesives intended for food contact applications."

Environmental Impact

Irganox® 1035 does not readily degrade in the environment. Toxicity to aquatic organisms is observed only at doses that exceed the solubility of this compound in water. Further, this material appears to be nontoxic to mammals and nonmutagenic. This compound does have the potential to migrate from food-contact materials into fatty foods such as olive oil.

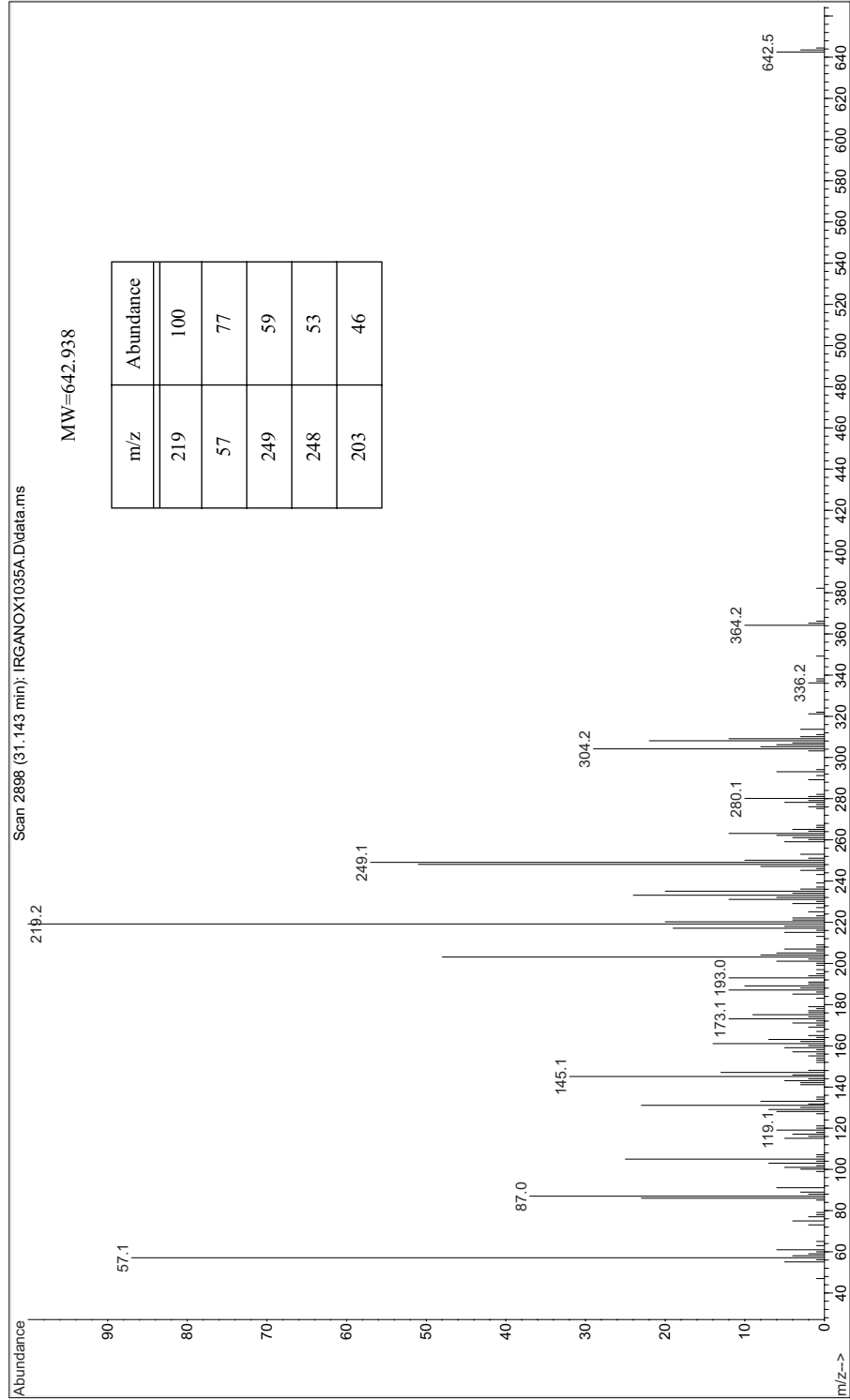
Point of Release

Major human exposure occurs only in the workplace, with consumer exposure being extraordinarily low.

Toxicological Data

Irganox® 1035 appears to be non-toxic through multiple routes (oral, dermal, and inhalation), with an oral LD50 greater than 5 g/kg [rat], and an acute dermal LD50 greater than 3 g/kg [rabbit], and an acute inhalation LD50 over 6.3 g/m³ [rat]. Subchronic further supports its non-toxic characteristics; NOELs have been calculated from 60 to 10,000 ppm in rats and dogs. These studies included a histological examination of all internal organs that showed no significant toxic effects.

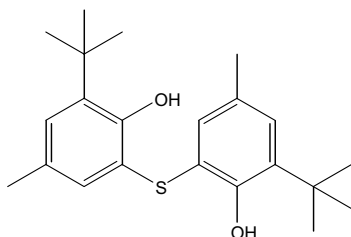
Mass Spectrum for Irganox® 1035 - PLAS-AX-069



For Chromatogram See Appendix A - PLAS-AX-069 - page 491

Irganox® 1081

Ciba Specialty Chemicals

**CAS Number** 90-66-4**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₂H₃₀O₂S**Molecular Weight** 358.54**Chemical Name**

6,6'-di-tert-butyl-2,2'-thiodi-p-cresol

Synonyms

2,2'-thiobis[6-(1,1-dimethylethyl)-4-methylphenol]; 2,2'-dihydroxy-3,3'-di-tert-butyl-5,5'-dimethyldiphenyl-sulfide; bis(5-methyl-3-tert-butyl-2-hydroxyphenyl) monosulfide

Brand Names & Manufacturers

Rionox 2246S

Rionlon Chemical Co.

Physical Properties**Appearance** White to light-yellow crystalline powder**Melting Point** 81-86 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH 35	EtOH U	Acetone >50	CH₂Cl₂ >50	Hexane 28
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Application *Application, Regulatory & Environmental Information*

Sulfur containing, high performance primary (phenolic) antioxidant and heat stabilizer used for the base stabilization of polyethylene wire and cable resins.

Regulatory Information

FDA approved for use in food contact applications.

Environmental Impact

Estimated log Pow >6 would indicate the potential for this chemical to bioaccumulate. It is not readily biodegradable and is considered to be toxic to aquatic organisms.

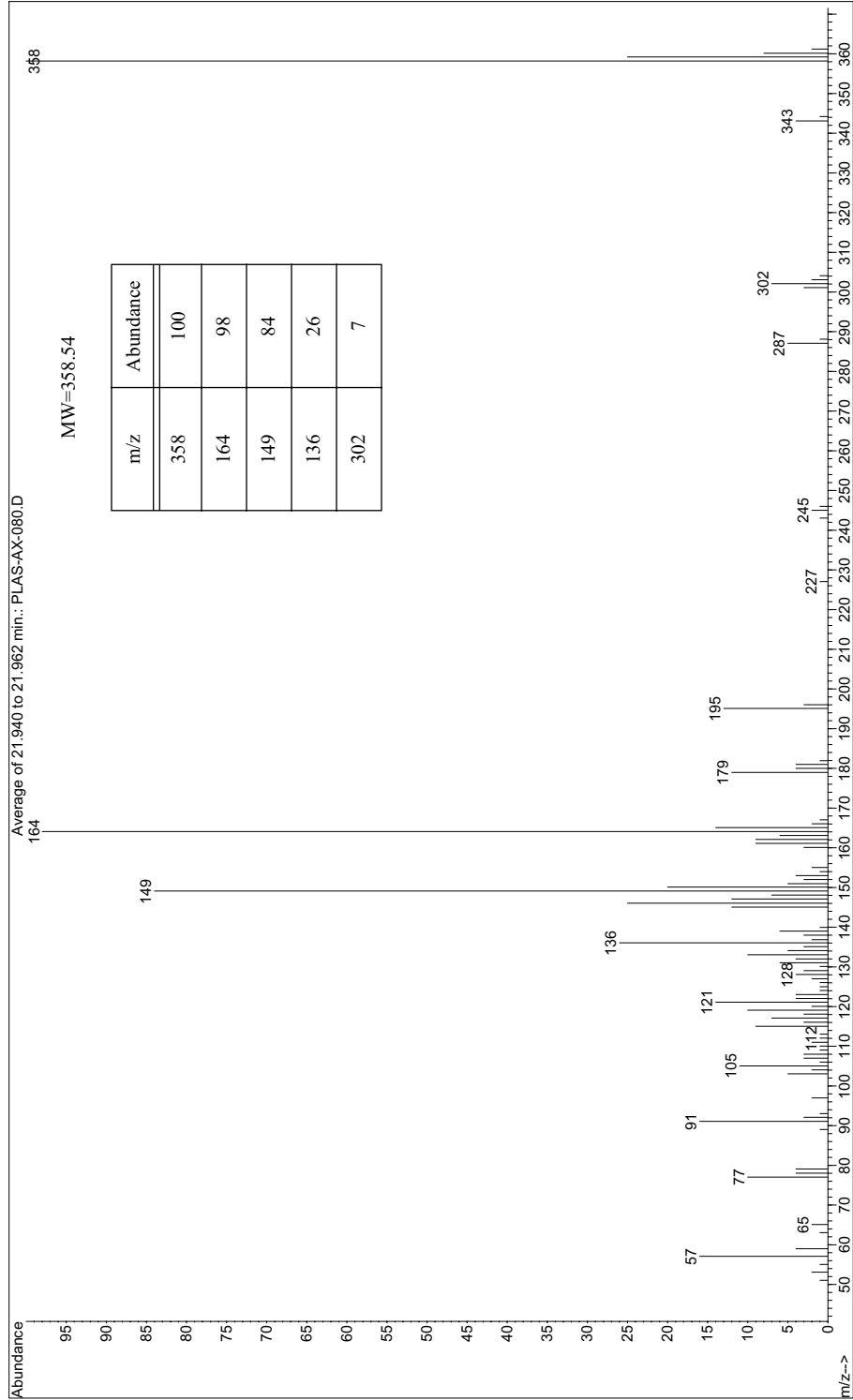
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

The toxicological properties of this material have not been fully determined.

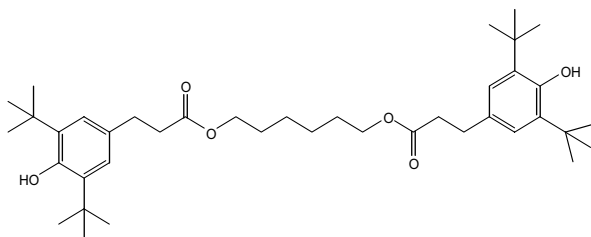
Mass Spectrum for Irganox® 1081 - PLAS-AX-080



For Chromatogram See Appendix A - PLAS-AX-080 - page 492

Irganox® 259

Ciba Specialty Chemicals

**CAS Number** 35074-77-2**RTECS Number** DA8342450**Abbreviation** Not Identified**Formula** C₄₀H₆₂O₆**Molecular Weight** 638.92**Chemical Name**

hexamethylene bis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate)

Synonyms

hexamethylene bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate); 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, 1,6-hexanediyl ester

Brand Names & Manufacturers

Irganox 259

Ciba Specialty Chemicals

Physical Properties**Appearance** White to off-white crystalline powder**Melting Point** 104-108 °C**Boiling Point** 654.4 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	1.7	U	36	U	1.5

Application, Regulatory & Environmental Information**Application** Irganox® 259 is a stabilizer for a wide range of thermoplastics, thermosets, synthetic fibers, and elastomers.**Regulatory Information**

FDA approved for the following applications: polymers, resins, or adhesives intended for food contact applications under 21CFR178.2010 and lubricants with incidental food contact.

Environmental Impact

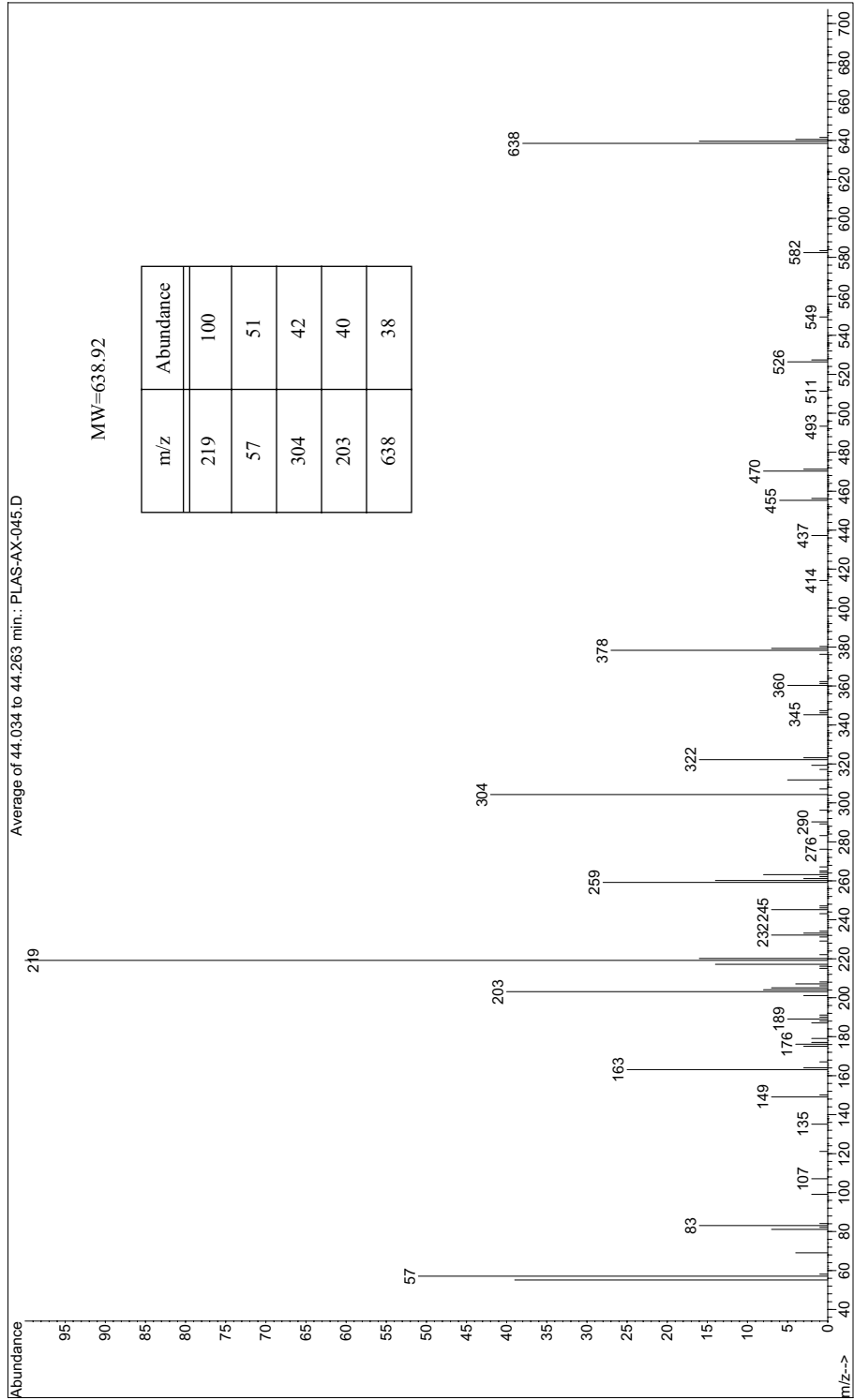
The low water solubility of the material makes it unlikely that hydrolysis would be a significant route of environmental degradation. Environmental accumulation is likely to occur in sediment and not in water.

Point of Release

Release can occur during manufacturing and shipping. Release may also occur from leaching from finished products especially in the presence of fatty esters.

Toxicological DataLowest published toxic oral dose (TDLo): 45500 mg/kg/13W-I [rat]; (LC50 96 h): > 100 mg/L [Fish]; (EC50 0–72 h): > 100 mg/L [Aquatic Plants]; (EC50 24 h) > 100 mg/L [Aquatic Invertebrates]; oral (LD50): > 7750 mg/kg [Mouse], > 10,000 mg/kg [Rabbit]; inhalation (LD50) > 1700 mg/m³ [Rat].

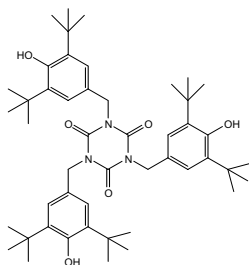
Mass Spectrum for Irganox® 259 - PLAS-AX-045



For Chromatogram See Appendix A - PLAS-AX-045 - page 493

Irganox® 3114 FF

Ciba Specialty Chemicals

**CAS Number** 27676-62-6**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₄₈H₆₉N₃O₆**Molecular Weight** 784.08**Chemical Name**

1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione

Synonyms1,3,5-tris((3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl)methyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione;
Tris(3,5-di-t-butyl-4-hydroxybenzyl) isocyanurate**Brand Names & Manufacturers**

Cyanox® 1741

Ethanox® 314

Vanox® GT

Cytec Technology Corp.

Albemarle Corporation

R.T. Vanderbilt Company, Inc.

Physical Properties**Appearance** White crystalline powder.**Melting Point** 218-220 °C**Boiling Point** 961 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	0.5	1.5	29	U	0.6

Application, Regulatory & Environmental Information

Application High molecular weight hindered phenolic antioxidant with photo and thermo-stability. Provides low volatility and resistance to extraction from polymer compounds. Suitable for PP, PE, polystyrene, ABS, PVC, nylon, and polyurethane. Also used as a radical scavenger providing stabilization for polyolefins.

Regulatory Information

FDA approved for use in various polymers and adhesives intended for food contact applications as defined in 21CFR178.2010 and 175.105.

Environmental Impact

Ecotoxicology data indicates that there is low concern for acute toxicity to fish, aquatic plants, and aquatic invertebrates. The data indicate that the material is not readily biodegradable; however, due to the low water solubility, environmental exposures are expected to be low. There is a low potential for bioaccumulation.

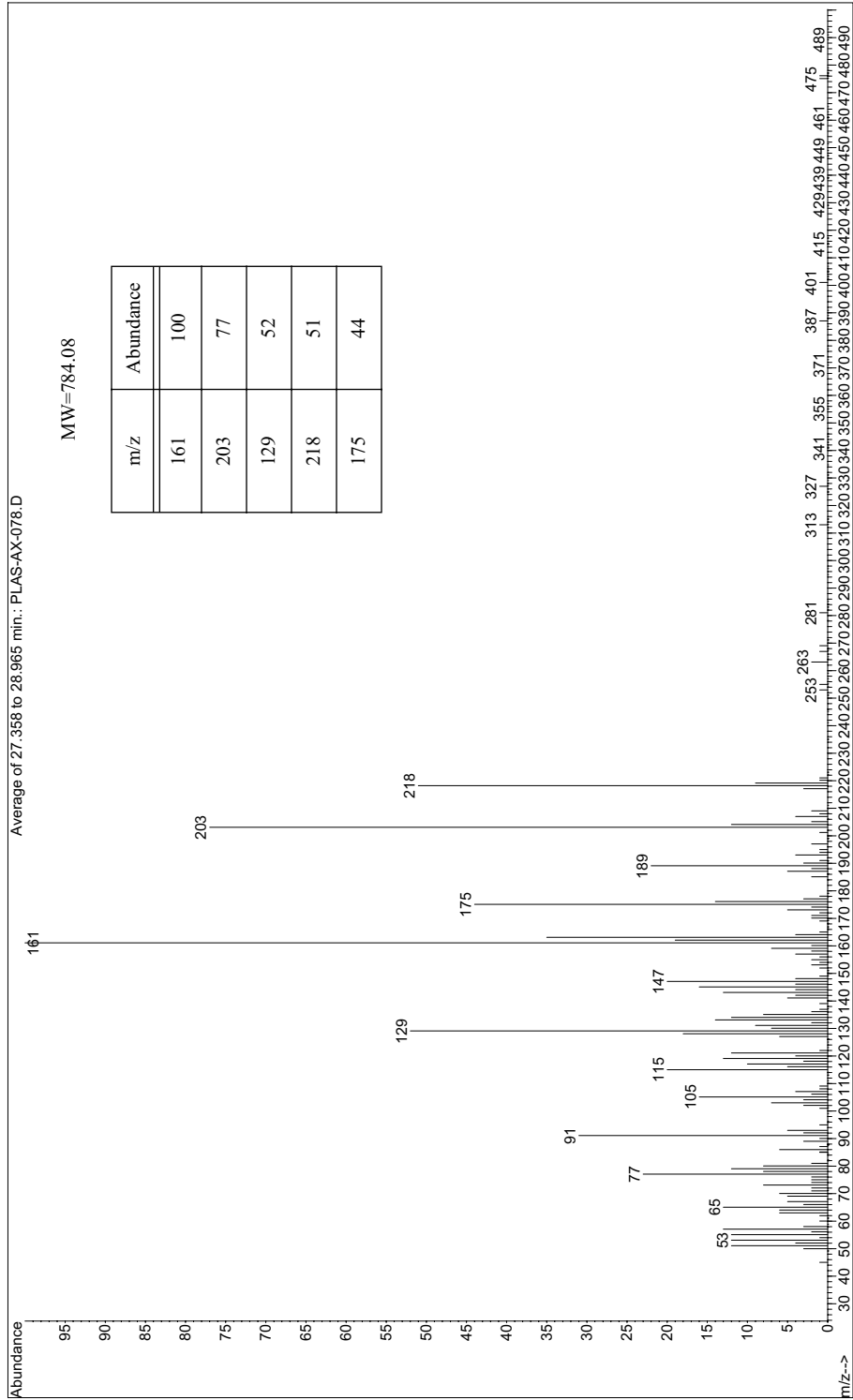
Point of Release

Can be released as point source pollution during manufacture, shipping, and use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

This substance was found to be neither carcinogenic nor a reproductive toxicant. Acute oral toxicity (LD50): >5000 mg/kg [Rat], acute dermal toxicity (LD50): >2000 mg/kg [Rat], acute toxicity of the dust (LC50): 270000 mg/m³ 4 hour [Rat].

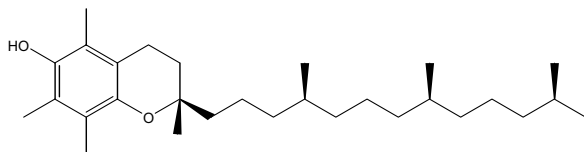
Mass Spectrum for Irganox® 3114 FF - PLAS-AX-078



For Chromatogram See Appendix A - PLAS-AX-078 - page 494

Irganox® E 201

Ciba Specialty Chemicals

**CAS Number** 10191-41-0**RTECS Number** GA8746000**Abbreviation** Not Identified**Formula** C₂₉H₅₀O₂**Molecular Weight** 430.71**Chemical Name**

alpha-tocopherol

Synonyms

vitamin E; ephanyl; 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol;
2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol

Brand Names & Manufacturers

Ciba Specialty Chemicals

Physical Properties**Appearance** Brown to yellow viscous oil**Melting Point** 3 °C**Boiling Point** 200-220 °C at 0.1 mmHg**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH >80	Acetone >80	CH₂Cl₂ >80	Hexane U
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Application, Regulatory & Environmental Information

Application Can be used for the stabilization of polyethylene for food and medical packaging applications. Can aid in melt flow and color control during processing.

Regulatory Information

FDA classified as Generally Recognized as Safe (GRAS). Approved in many different countries for food applications.

Environmental Impact

This product and its degradation products are not expected to have any negative effects on the environment.

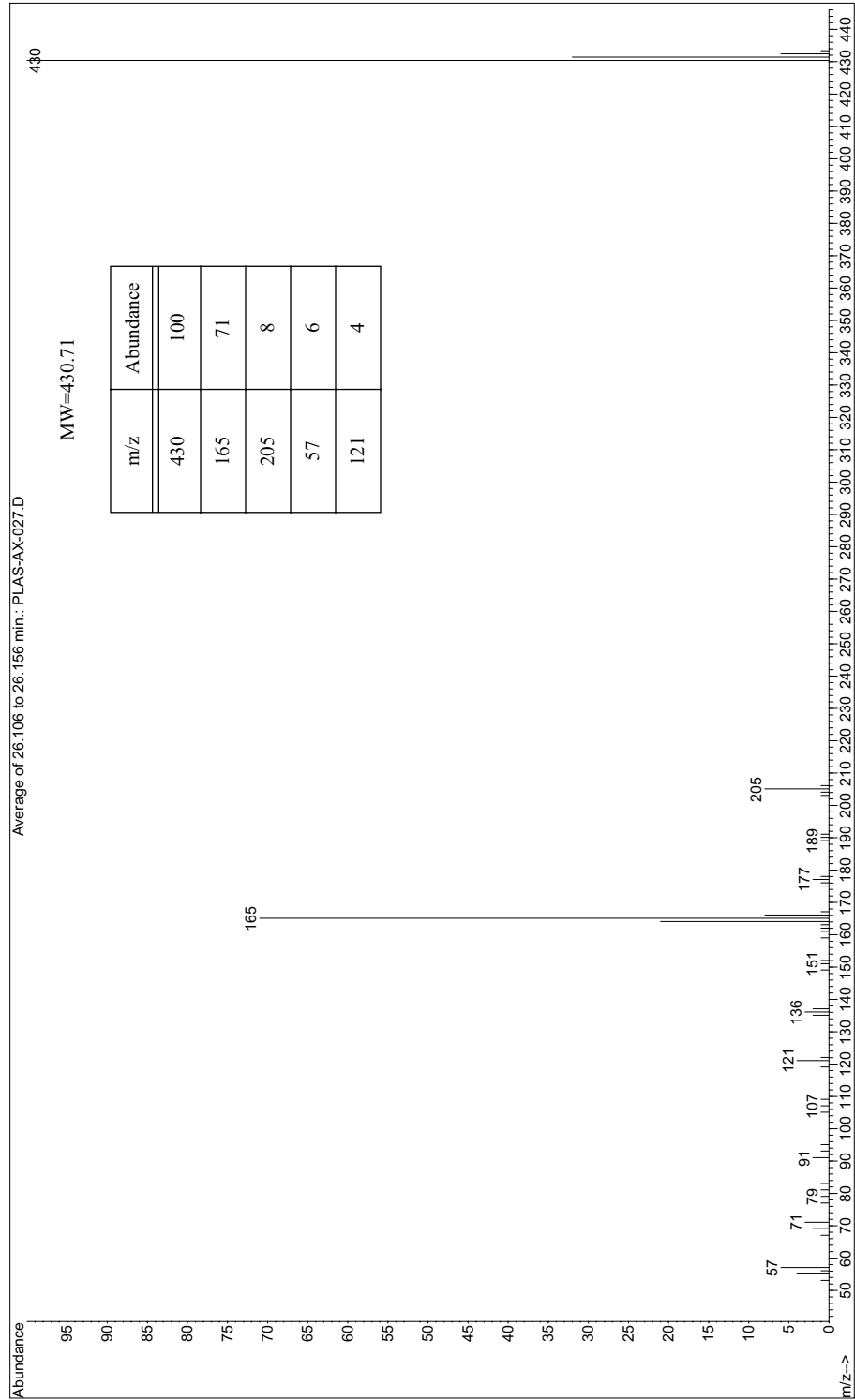
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Vitamin E has not been associated with affecting genetic material or adverse reproductive effects in humans; however, when Vitamin E was given to mice in large doses, it was associated with growth retardation of the fetus and an increase in cleft palate. Furthermore, it did affect the genetic material of lab rats when doses of 2500 µg/kg were administered intraperitoneally. Acute oral toxicity (LD50): >4000 mg/kg [Mouse].

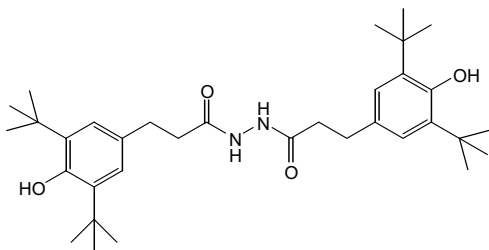
Mass Spectrum for Irganox® E 201 - PLAS-AX-027



For Chromatogram See Appendix A - PLAS-AX-027 - page 495

Irganox® MD 1024

Ciba Specialty Chemicals

**CAS Number** 32687-78-8**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₃₄H₅₂N₂O₄**Molecular Weight** 552.79**Chemical Name**

1,2-bis(3,5-di-tert-butyl-4-hydroxyphenyl)hydrazide

Synonyms

2',3-bis((3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionyl))propionohydrazide

Brand Names & Manufacturers

Lowinox® MD24

Chemtura Corporation

Physical Properties**Appearance** White to slightly yellowish crystalline powder**Melting Point** 227-232 °C**Boiling Point** 742 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	4	U	4	U	<0.01

Application, Regulatory & Environmental Information

Application Metal deactivator that acts as a hindered phenolic antioxidant. Used in conjunction with phenolic antioxidants, phosphites/phosphonites, thio-synergists, and other co-additives. Most suited for PA, PE, rubbers, and PP applications.

Regulatory Information

Irganox® MD 1024 is approved by the FDA for use in packaging polymers, resins, and adhesives intended for food contact applications. It is approved in many countries for food contact applications.

Environmental Impact

After this material is incorporated in the polymer matrix it is relatively immobile and release/exposure to humans or the environment is considered minimal. Under environmental conditions, the low solubility of the material should preclude the occurrence of acutely toxic exposures. The compound has very low volatility, and a calculated log Pow of >6. Based on its properties it is likely to bind to the soil and sediment where it is expected to be immobile and have limited bioavailability.

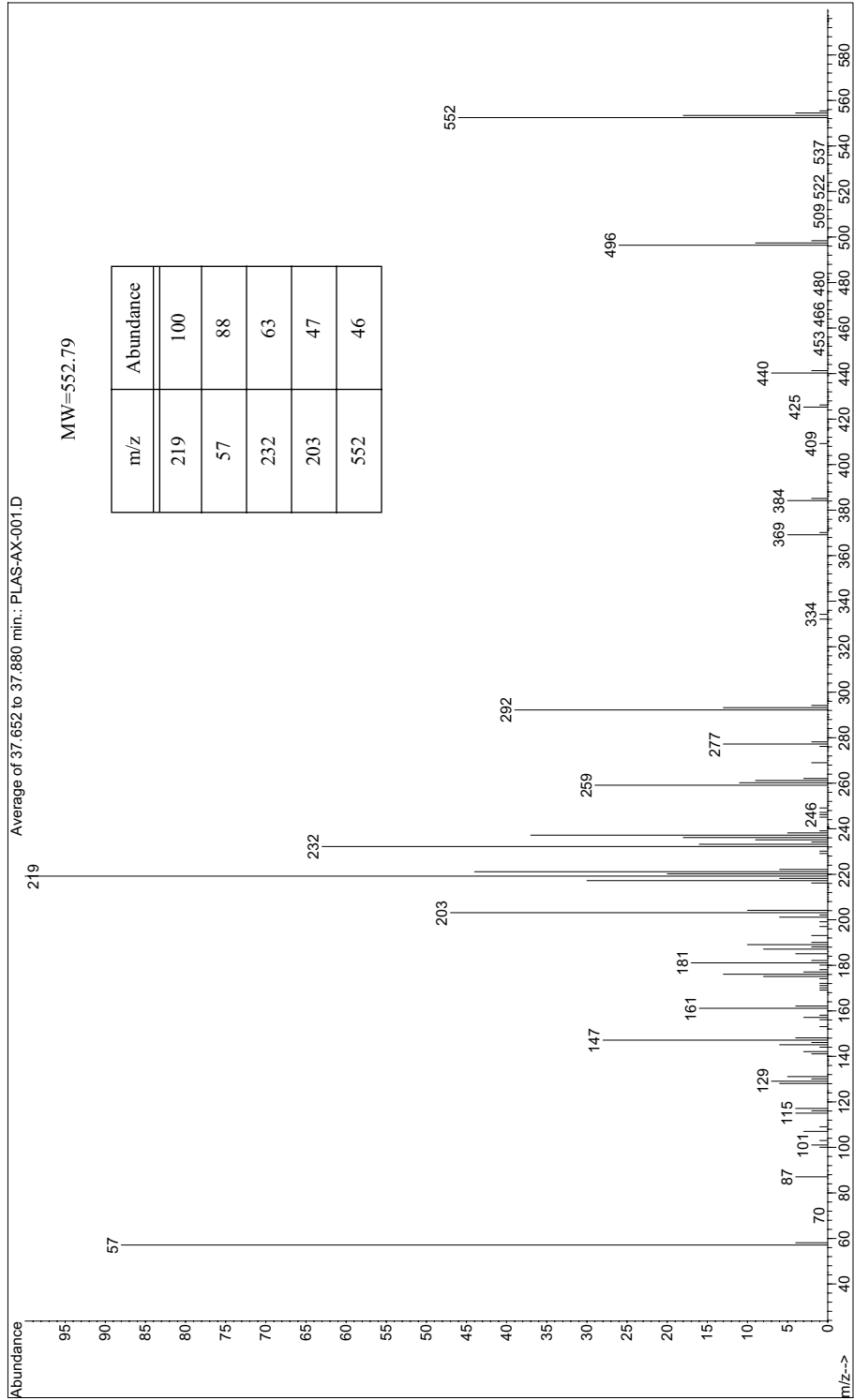
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Available mammalian acute toxicity data indicates very low toxicity by oral or inhalation exposure. It is neither teratogenic nor embryotoxic and it does not impact reproductive organs, even at relatively high exposure levels. Additionally, the compound is not mutagenic or clastogenic. In a subchronic 28-day toxicity study in the rat, there are no adverse effects up to 1000 mg/kg BW per day.

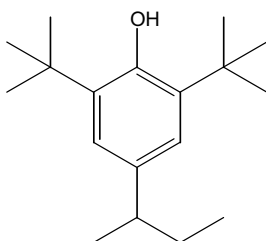
Mass Spectrum for Irganox® MD 1024 - PLAS-AX-001



For Chromatogram See Appendix A - PLAS-AX-001 - page 496

Isonox® 132

SI Group Incorporated

**CAS Number** 17540-75-9**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₁₈H₃₀O**Molecular Weight** 262.43**Chemical Name**

2,6-di-tert-butyl-4-sec-butylphenol

Synonyms

4-sec-butyl-2,6-di-tert-butylphenol

Brand Names & Manufacturers

Isonox® 132

SI Group Incorporated

Physical Properties**Appearance** Clear liquid**Melting Point** ~25 °C**Boiling Point** 275 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application** Phenolic antioxidant for polyols, PVC, and adhesives.**Regulatory Information**

FDA approved for food contact use in PVC not to exceed 0.06% by weight of the finished product.

Environmental Impact

Log Kow value of 6.43. Since it is relatively insoluble in water, primary accumulation anticipated in the sediment. This material is estimated to be aerobically degradable, with primary degradation in occurring weeks, and complete degradation in months. (LC50 96 hour): 0.072 mg/L [Fish], (LC50 48 hour): 0.22 mg/L [Daphnia].

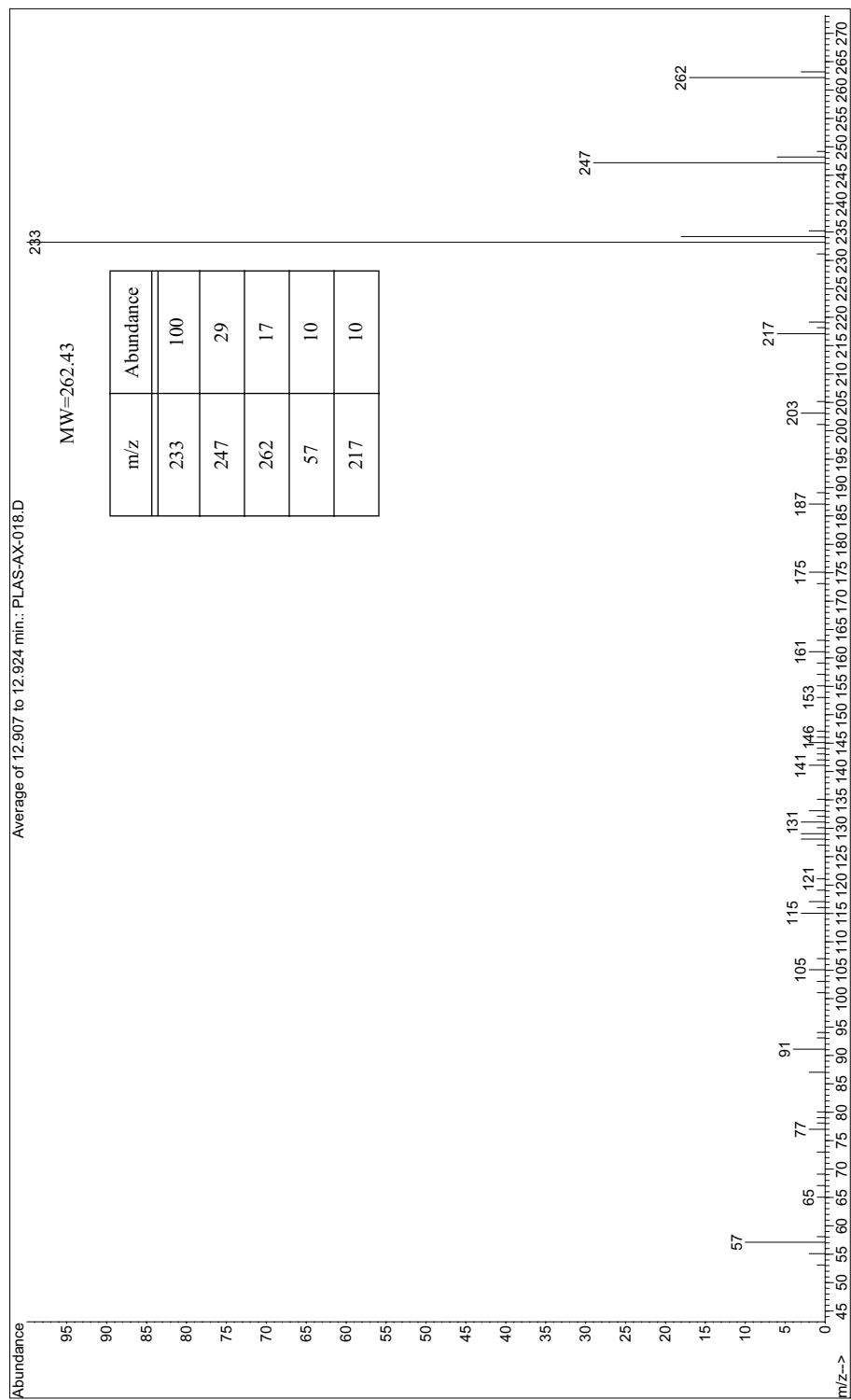
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

May cause respiratory or skin sensitization. Acute oral toxicity (LD50): 2000 mg/kg [Rat].

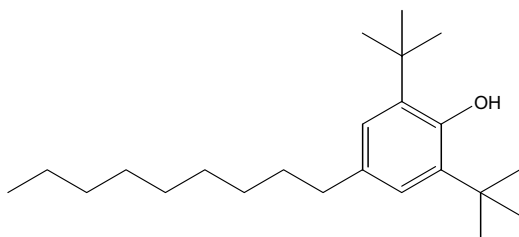
Mass Spectrum for Isonox® 132 - PLAS-AX-018



For Chromatogram See Appendix A - PLAS-AX-018 - page 497

Isonox® 232

SI Group Incorporated

**CAS Number** 4306-88-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₃H₄₀O**Molecular Weight** 332.57**Chemical Name**

2,6-di-tert-butyl-4-nonylphenol

Synonyms

2,6-bis(1,1-dimethylethyl)-4-nonylphenol

Brand Names & Manufacturers

IonoI® 926

Degussa

Physical Properties**Appearance** Colorless to light-yellow liquid with a mild, aromatic odor**Melting Point** >5 °C**Boiling Point** 335-345 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application **Application, Regulatory & Environmental Information**

Phenolic antioxidant for polyol and polyurethane foam. Also used as a lubricating oil additive.

Regulatory Information

No information available.

Environmental Impact

Aquatic toxicity: (LC50): >10 mg/L/96 hour [Rainbow trout]. Material can biodegrade (BOD28 ~30%).

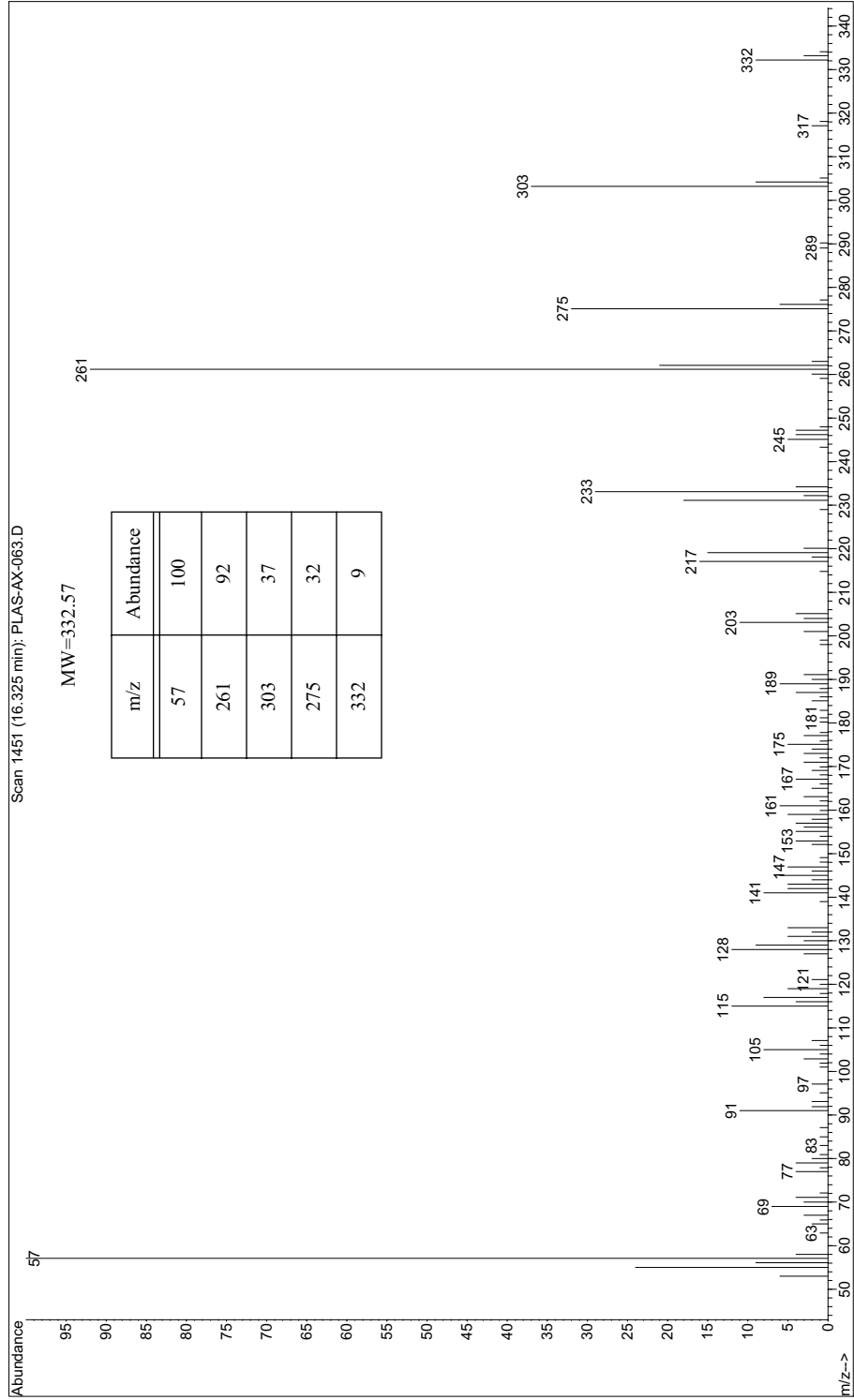
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

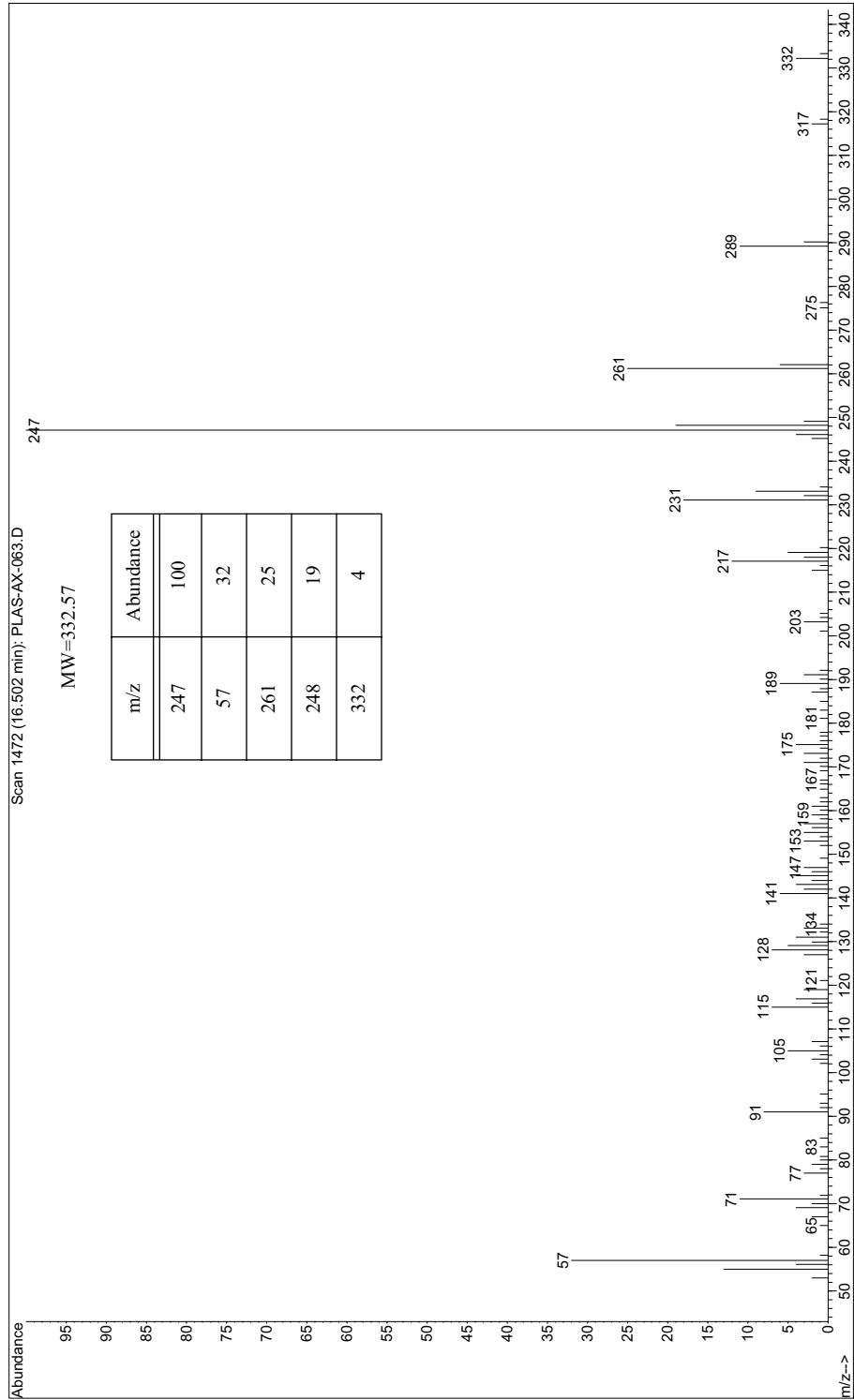
Acute oral toxicity (LD50): >2000 mg/kg [Rat].

Mass Spectrum for Isonox® 232 - PLAS-AX-063



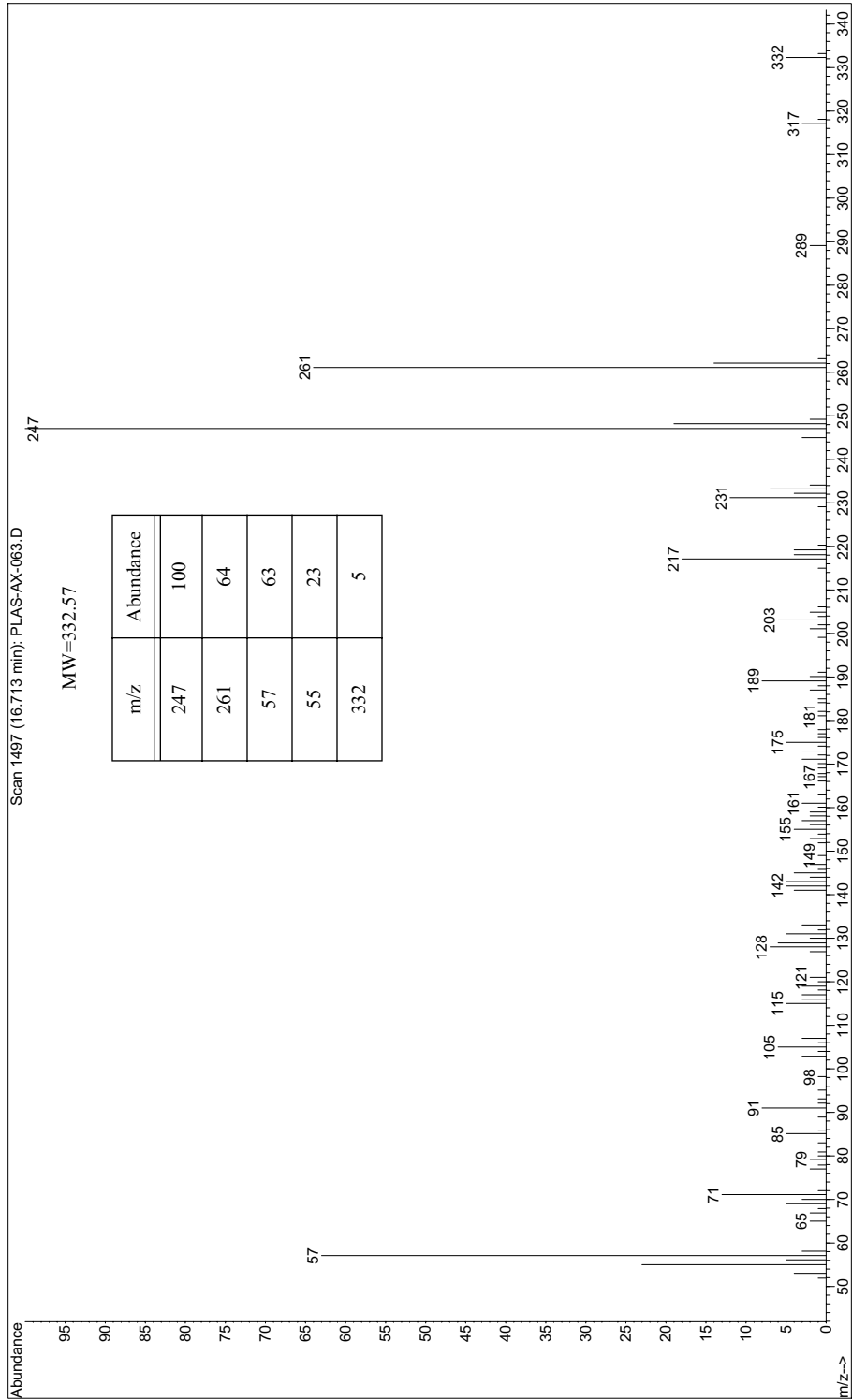
For Chromatogram See Appendix A - PLAS-AX-063 - page 498

Mass Spectrum for Isonox® 232 - PLAS-AX-063



For Chromatogram See Appendix A - PLAS-AX-063 - page 498

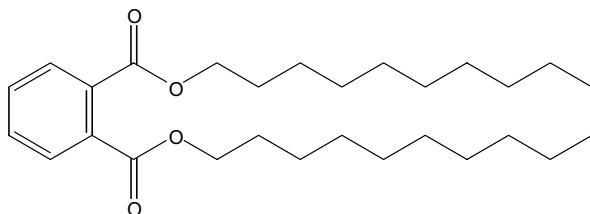
Mass Spectrum for Isonox[®] 232 - PLAS-AX-063



For Chromatogram See Appendix A - PLAS-AX-063 - page 498

Lowinox® AH25

Chemtura Corporation

**CAS Number** 79-74-3**RECS Number** MX6300000**Abbreviation** Not Identified**Formula** C₁₆H₂₆O₂**Molecular Weight** 250.38**Chemical Name**

2,5-bis(1,1-dimethylpropyl)-1,4-benzenediol

Synonyms

2,5-di-tert-pentylhydroquinone; 2,5-bis(1,1-dimethylpropyl)hydroquinone; 2,5-di-tert-amylhydroquinone

Brand Names & Manufacturers

Antioxidant 250-SVA

Akrochem Corporation

Physical Properties**Appearance** White to cream powder or granules; odorless**Melting Point** 177-184 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	68	72	U	U

Application, Regulatory & Environmental Information**Application**

Lowinox® AH25 is a phenolic antioxidant that reduces cold flow in unvulcanized rubber and protects against sun cracking. Also slows the skinning (drying out) of paint resins and adhesive coating; extends tack in uncured adhesives, tapes, and hot-melt adhesives at up to a 0.5 to 4.0 phr level.

Regulatory Information

FDA approved 1998 for the following applications: adhesives in safe contact with food in all stages of production, processing, and packaging; adhesives, 21CFR175.105; in the manufacture of rubber material intended for use in all stages of production, processing, packaging, and transport of food, 21CFR177.2600.

Environmental Impact

Not readily biodegradable. Hazardous to the environment and toxic to aquatic organisms. (EC50 24 hour): 0.91 mg/L [Daphnia]; (LC50 96 hour): 0.067 mg/L [Trout], 34 µg/L [Bluegill], 0.12 mg/L [Fathead minnow]; (LC50 48 hour): 35 µg/L [Bluegill]; (LC50 24 hour): 42 µg/L [Rainbow trout], 49 µg/L [Bluegill]; (EC50 96 hour): 1.7 ppm [Selenastrum capricornutum].

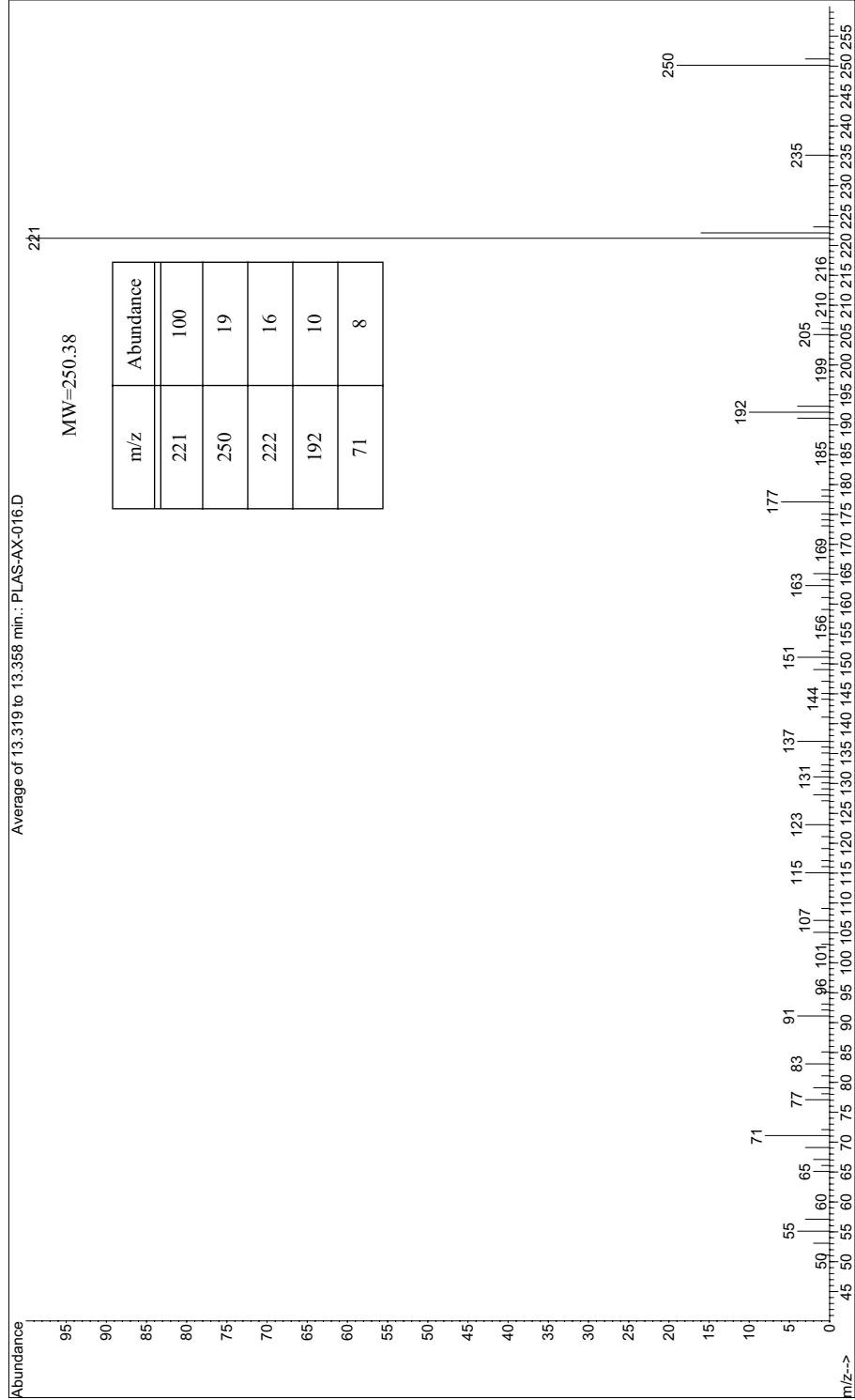
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

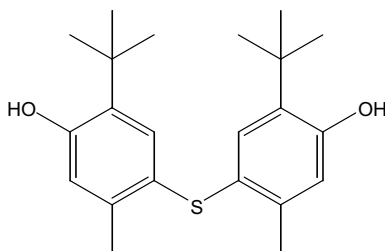
Toxicological Data

The toxicological properties of this material have not been thoroughly investigated. Not listed (ACGIH, IARC, NTP, OSHA) as a cancer-causing agent. Acute intraperitoneal (LD50): 200 mg/kg [Mouse]; acute dermal (LD50): >3160 mg/kg [Rabbit]; acute oral (LD50): 2 g/kg [Rabbit], 1900 mg/kg [Rat].

Mass Spectrum for Lowinox® AH25 - PLAS-AX-016



For Chromatogram See Appendix A - PLAS-AX-016 - page 499

Lowinox® TBM-6

CAS Number 96-69-5
RTECS Number GP3150000
Abbreviation TBBC

Formula C₂₂H₃₀O₂S
Molecular Weight 358.54

Chemical Name

4,4'-thiobis(2-tert-butyl-5-methylphenol)

Synonyms

bis(3-tert-butyl-4-hydroxy-6-methylphenyl)sulfide; 4,4'-thiobis(6-tert-butyl-3-methylphenol); 1,1-thiobis(2-methyl-4-hydroxy-5-tert-butylbenzene)

Brand Names & Manufacturers

Cyanox® 1760	Cytec Technology Corp.
Santonox® TBMC	Flexsys America L.P.
Rhodianox TBM6 (P/T/TP)	Rhone-Poulenc Chimie Corp.

Physical Properties

Appearance	White to cream-colored crystalline powder; phenolic odor					
Melting Point	160-164 °C		Boiling Point Decomposes at 300 °C			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water 0.08	MeOH 79	EtOH 47	Acetone 20	CH₂Cl₂ U	Hexane ~0.75

Application, Regulatory & Environmental Information

Application
 TBM-6 is a hindered thiophenol antioxidant used in natural and synthetic rubbers with high thermo-oxidative degradation resistance properties. It is a polymerization and processing "light-stabilizer" in PP, ABS, PVC, EPDM, polybutadienes and in HDPE/LDPE (for tubes, gas pipe connectors, high voltage cables, and films for food packaging applications). TBM-6 is also a heat stabilizer for lubricants, an anti-skinning agent for hot melt adhesives, and an anti-scorching agent for polyurethanes. Exhibits compatibility with peroxides and in tandem with carbon black.

Regulatory Information

FDA approved 1998 for the following applications: in the manufacture of antioxidants/stabilizers for polymers intended for use in all stages of production, processing, packaging, and transport of food: 21CFR part 178.2010. UK approved 1992 as an antioxidant for materials composed of PE and PP in contact with water or food intended for human consumption up to 0.25% of the final product composition.

Environmental Impact

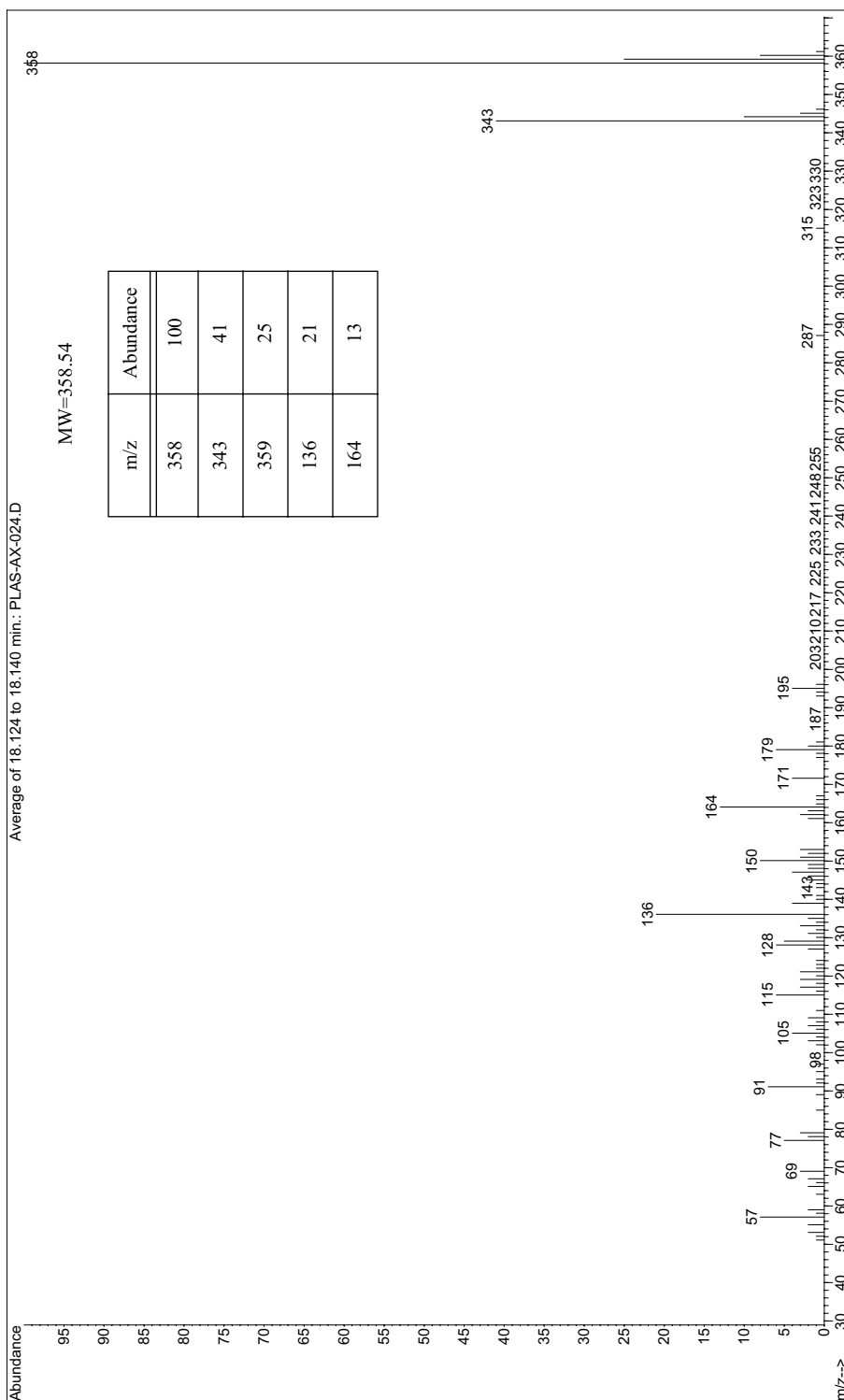
Not readily biodegradable. TBM-6 lacks a hydrolyzable functional group, and therefore undergoes slow degradation. Toxic to aquatic organisms. (LC50 96 hour): 0.24 mg/L [bluegill sunfish]; (EC50 24 hour): 0.23 mg/L [Daphnia Magna].

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

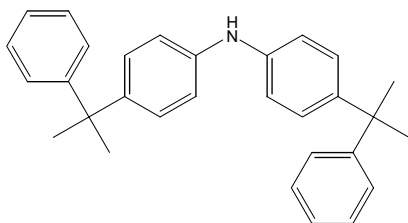
Not listed (ACGIH, IARC, NTP, OSHA) as a cancer-causing agent. TBM-6 is not mutagenic with or without metabolic activation. Acute intraperitoneal (LD50): 50 mg/kg [Mouse]; acute oral (LD50) 2345 mg/kg [Rat], 4750 mg/kg [Mouse], 3200 mg/kg [Rabbit]; acute dermal (LD50): >5010 mg/kg [Rabbit].

Mass Spectrum for Lowinox® TBM-6 - PLAS-AX-024

For Chromatogram See Appendix A - PLAS-AX-024 - page 501

Naugard® 445

Chemtura Corporation

**CAS Number** 10081-67-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₃₀H₃₁N**Molecular Weight** 405.57**Chemical Name**

4,4'-bis(alpha,alpha-dimethylbenzyl)diphenylamine

Synonyms

4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline; 4,4'-di-(alpha,alpha-dimethylbenzyl) diphenylamine

Brand Names & Manufacturers

Antioxidant 405

Akrochem Corporation

Physical Properties**Appearance** White powder or granules**Melting Point** 98-100 °C**Boiling Point** ~507 °C (estimated)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.7	U	40.8	U	0.7

Application**Application, Regulatory & Environmental Information**

Naugard® 445 is non-discoloring aromatic amine antioxidant that works synergistically with phosphites and phenolic antioxidants as a thermal stabilizer in polyolefins, styrenics, polyols, hot melt adhesives, lubricants, and polyamides.

Regulatory Information

FDA approved in food-contact surface of articles intended for use in the production, manufacturing, packing, processing, preparing, treating, packaging, transporting, or storage of food as defined in 21CFR175.300; as an antioxidant and/or stabilizer in polymers (not to exceed 0.3% weight of PP complying with 21CFR177.1520); and in PP (with non-fatty foods only) as defined in 21CFR178.2010.

Environmental Impact

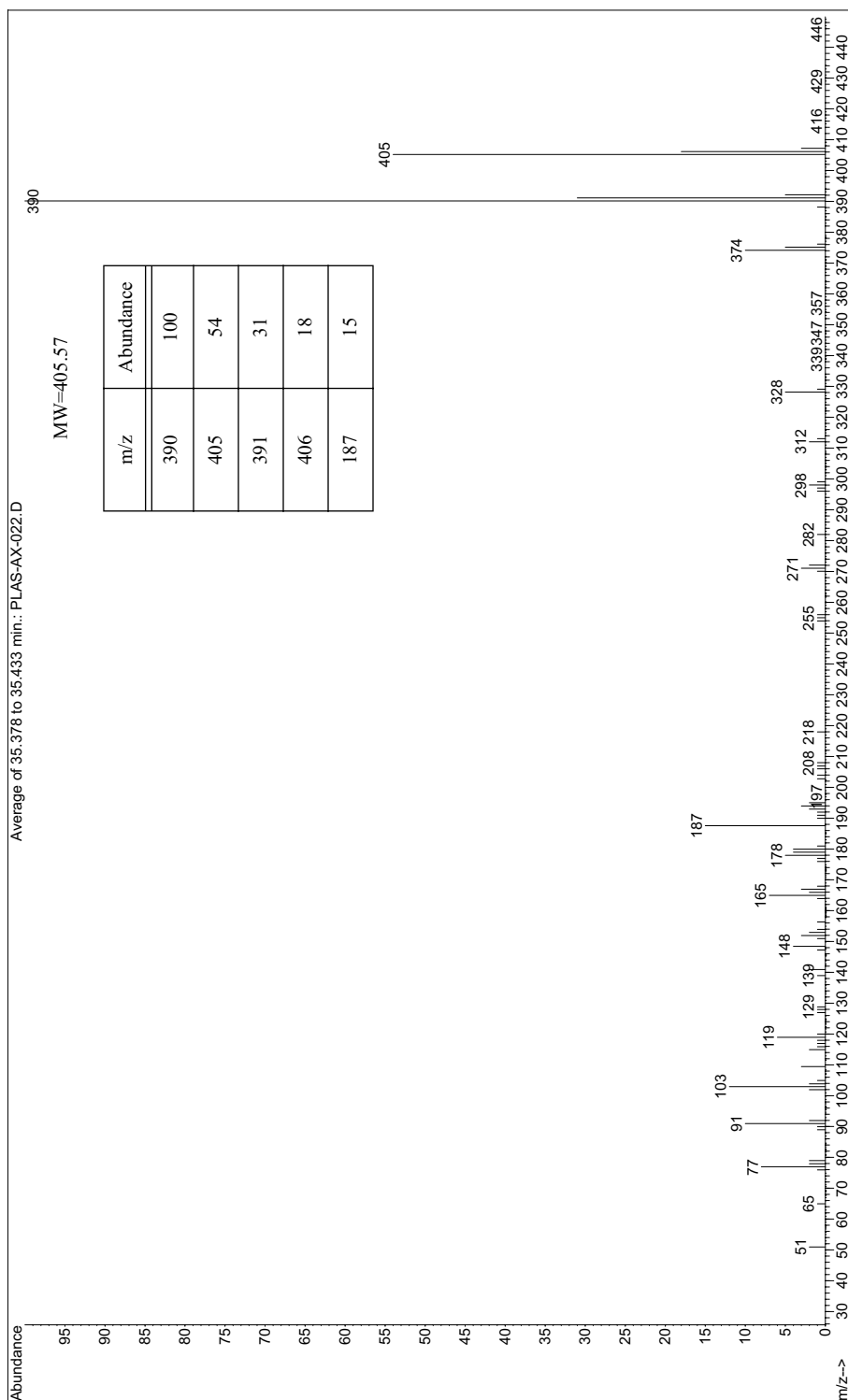
Not readily biodegradable. Log Pow value = 8.51, indicates a high potential to bioaccumulate in aquatic organisms. Direct photolysis t(1/2) 0.6 hrs. Ecotoxicity: (LC50 96 hour): 0.23 µg/L [Fish]; (EC50 48 hour): 0.038 µg/L [Daphnia]; (EC50 96 hour): 0.349 µg/L [Aquatic Plants].

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

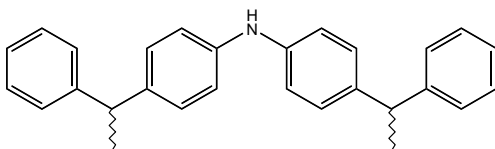
Not listed (ACGIH, IARC, NTP, OSHA) as a cancer-causing agent. Acute oral (LD50): >10 g/kg BW [Male Rat].

Mass Spectrum for Naugard® 445 - PLAS-AX-022

For Chromatogram See Appendix A - PLAS-AX-022 - page 502

Naugard 635

Chemtura Corporation

**CAS Number** 68442-68-2**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₈H₂₇N**Molecular Weight** 377.52**Chemical Name**

4-(1-phenylethyl)-N-[4-(1-phenylethyl)phenyl]aniline

Synonyms

Styrenated diphenylamine; Styrenated N-phenyl-benzenamine

Brand Names & Manufacturers

Westco AO-29

Western Reserve Chemical

Wingstay S

Physical Properties**Appearance** Light beige powder**Melting Point** 196 °C**Boiling Point** >300 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application**Application, Regulatory & Environmental Information**

Used as antidegradants in rubber, foamed polymers, and high-temperature functional fluids, and antioxidants in finished rubber articles.

Regulatory Information

FDA regulated for use as an indirect food additive - 21CFR §175.105 (adhesive components)

Environmental Impact

These materials have high estimated log Kow values, such that acute toxicity is not expected at or below their low levels of water solubility. Biodegradation: 9% after 28 days. BCF 9572 (estimated).

LC50 (fish): 920 mg/kg

Point of Release

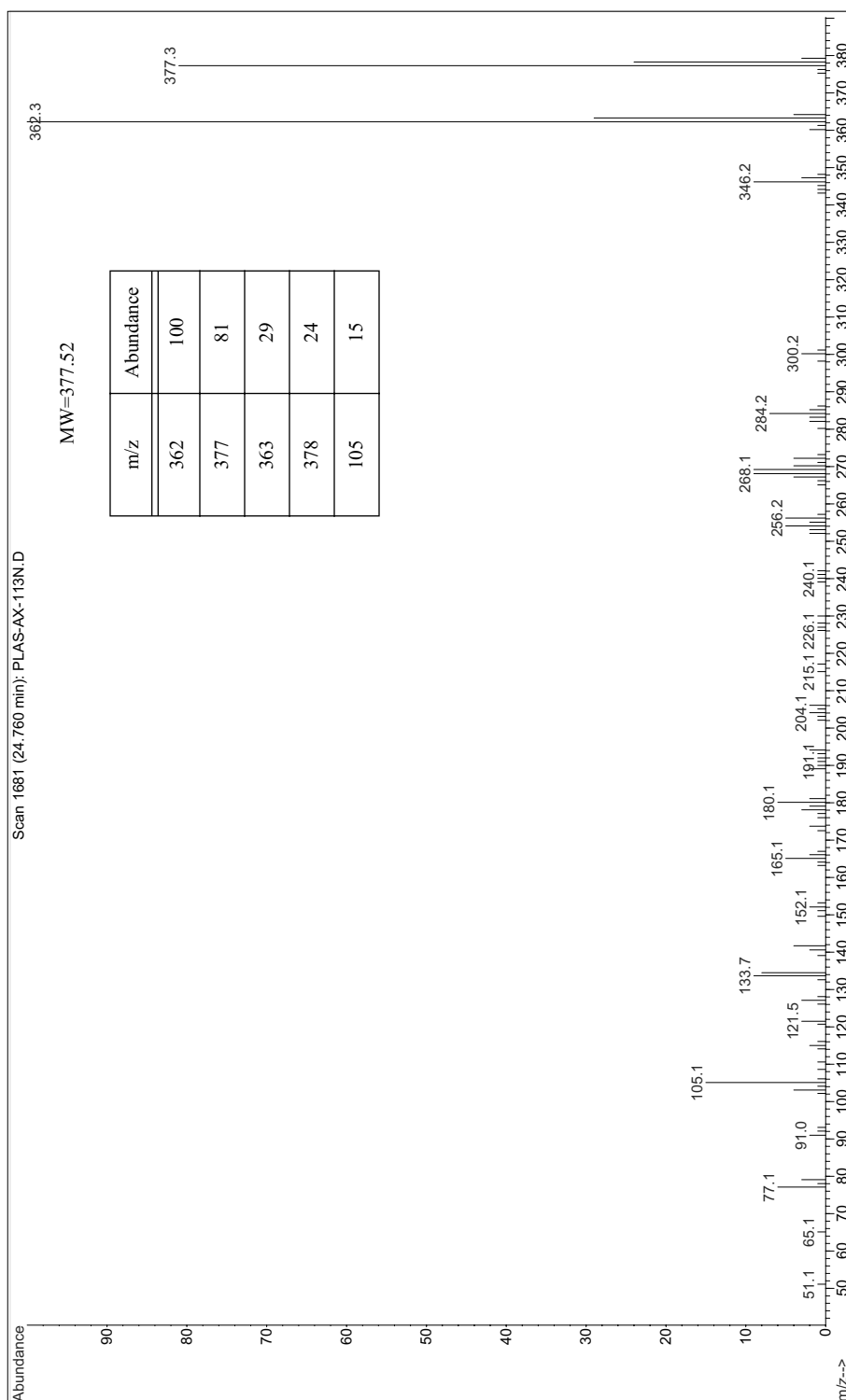
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

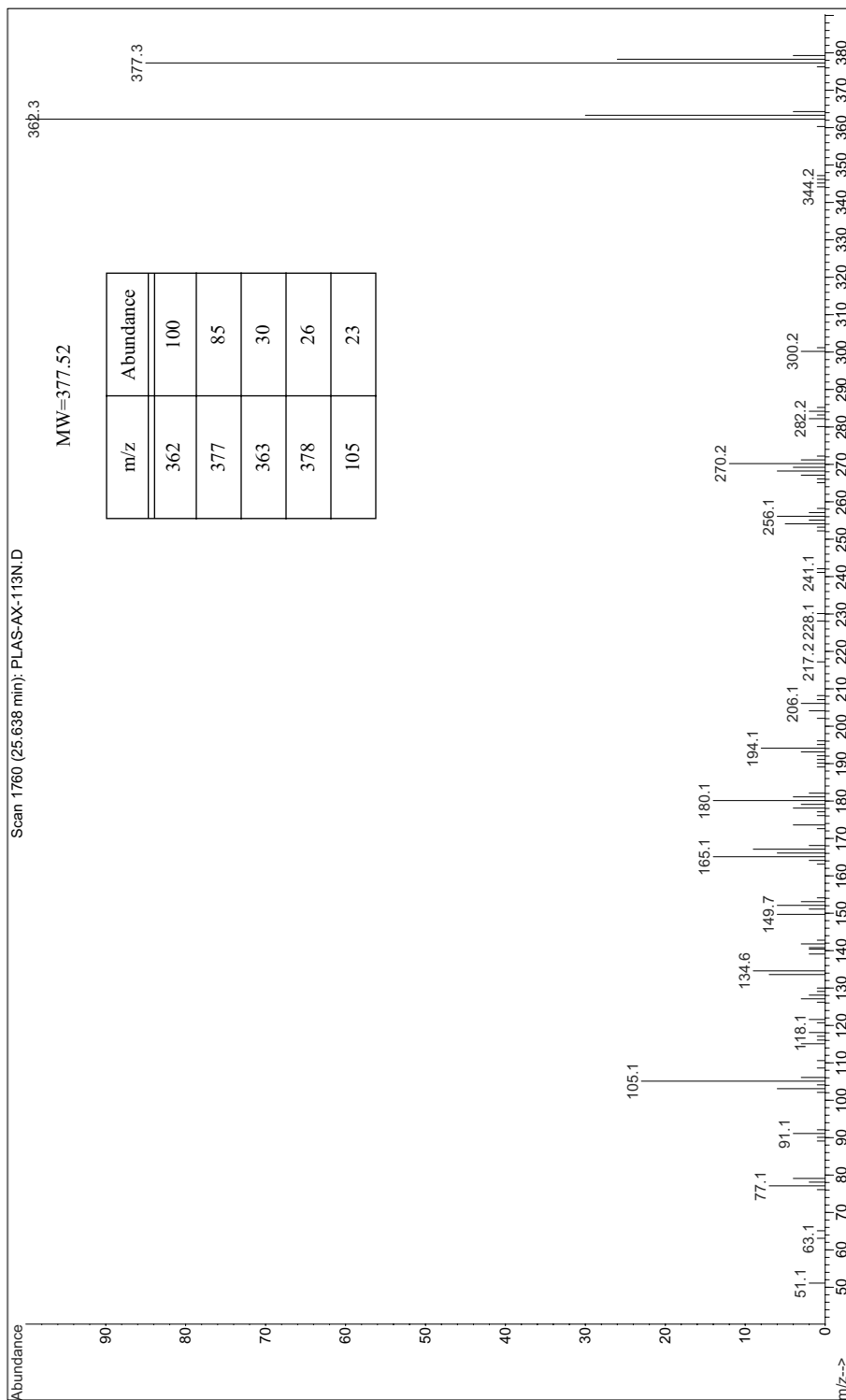
Mammalian toxicity — low concern for acute toxicity and mutagenicity.

Oral LD50: >20,000 mg/kg

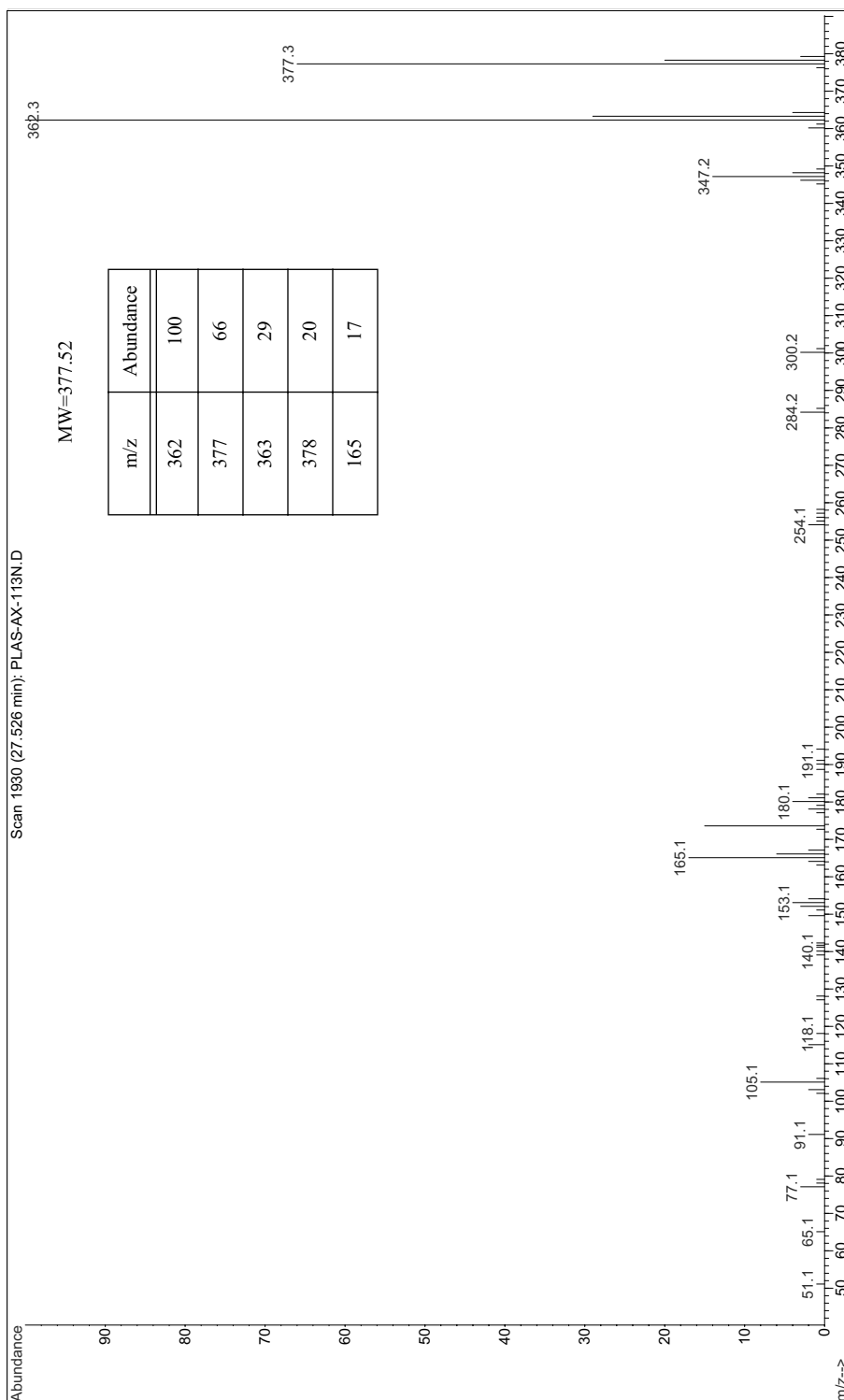
Dermal LD50: >10,000 mg/kg

Mass Spectrum for Naugard 635 - PLAS-AX-113

For Chromatogram See Appendix A - PLAS-AX-113 - page 503

Mass Spectrum for Naugard 635 - PLAS-AX-113

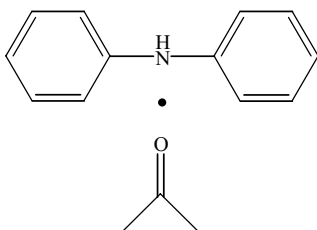
For Chromatogram See Appendix A - PLAS-AX-113 - page 503

Mass Spectrum for Naugard 635 - PLAS-AX-113

For Chromatogram See Appendix A - PLAS-AX-113 - page 503

Naugard® A

Chemtura Corporation



CAS Number 68412-48-6

RTECS Number UC3810000

Abbreviation Not Identified

Formula $C_{12}H_{11}N \cdot C_3H_6O$

Molecular Weight N/A

Chemical Name

acetone diphenylamine condensation products

Synonyms

2-propanone, reaction products with diphenylamine, ADPA

Brand Names & Manufacturers

AgeRite® Superflex®

RT Vanderbilt

Physical Properties**Appearance** Greenish-tan flake or powder**Melting Point** 85-95 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	U	40-80	U

Application**Application, Regulatory & Environmental Information**

Antioxidant for natural and synthetic rubber, tires, automotive and appliance molded goods, polyamides and carbon black filled olefin formulations for use in geomembranes, wire and cable jacketing, and irrigation piping.

Regulatory Information

Does not have FDA approval for use in food contact applications.

Environmental Impact

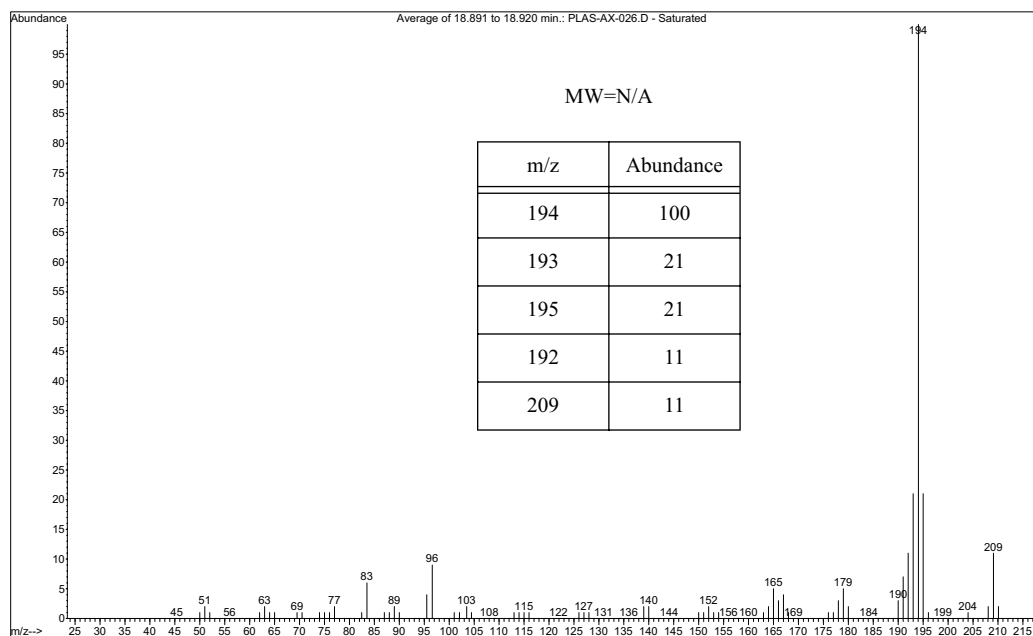
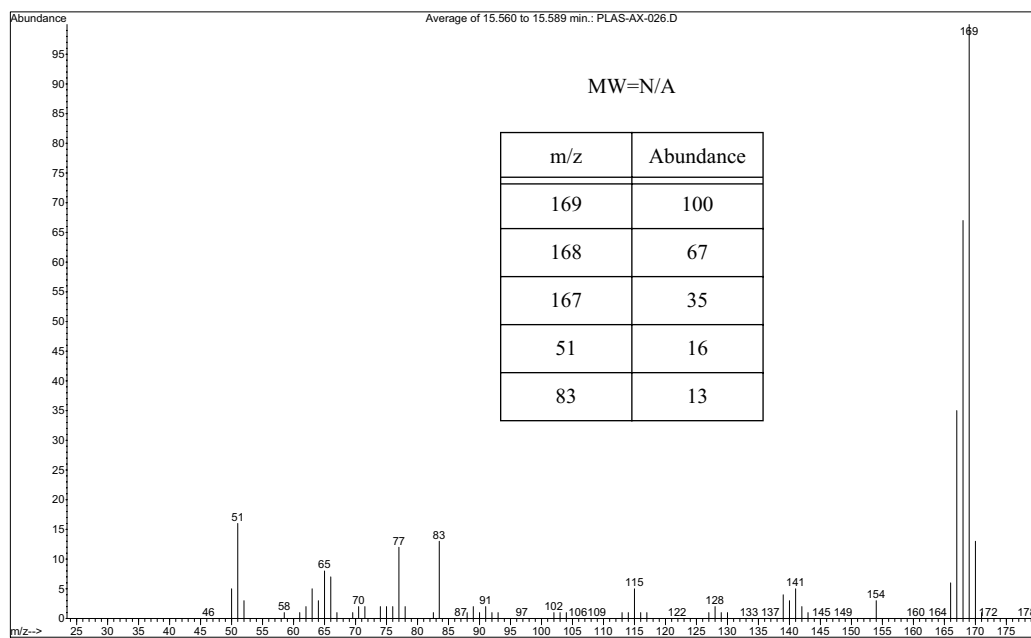
Classified as a persistent, bioaccumulative toxin and is inherently toxic to aquatic organisms.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

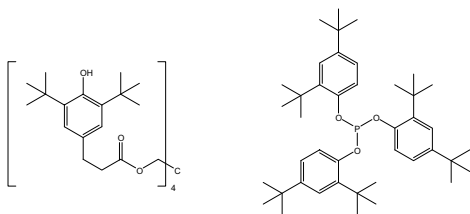
(LD50): > 10 g/kg oral, [Rat].

Mass Spectra for Naugard® A - PLAS-AX-026

For Chromatogram See Appendix A - PLAS-AX-026 - page 504

Naugard® B-25

Chemtura Corporation

 $C_{73}H_{108}O_{12}$ $C_{42}H_{63}O_3P$ **CAS Number** See below**RTECS Number** N/A**Abbreviation** Not Identified**Formula** See below structure**Molecular Weight** 1177.65/ 646.92**Chemical Name**

1:1 blend of Naugard® 10 and Naugard® 524

Synonyms

tris(2,4-di-tert-butylphenyl)phosphite and tetrakis methylene(3,5-di-tert-butyl-4-hydroxyhydrocinnamate) methane (1:1 blend)

Brand Names & Manufacturers

Naugard B-25

Chemtura Corporation

Physical Properties**Appearance** White to off-white powder or granules**Melting Point** Not available**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<0.1	U	U	55	<0.5

Application**Application, Regulatory & Environmental Information**

This compound is a blend of two compounds: CAS Numbers 6683-19-8 and 31570-04-4.

Antioxidant used for wood or other natural fiber-filled polyolefins, elastomers, and hot melt adhesives when light exposure and maintenance of color is important.

Regulatory Information

FDA approved for various food contact applications.

Environmental Impact

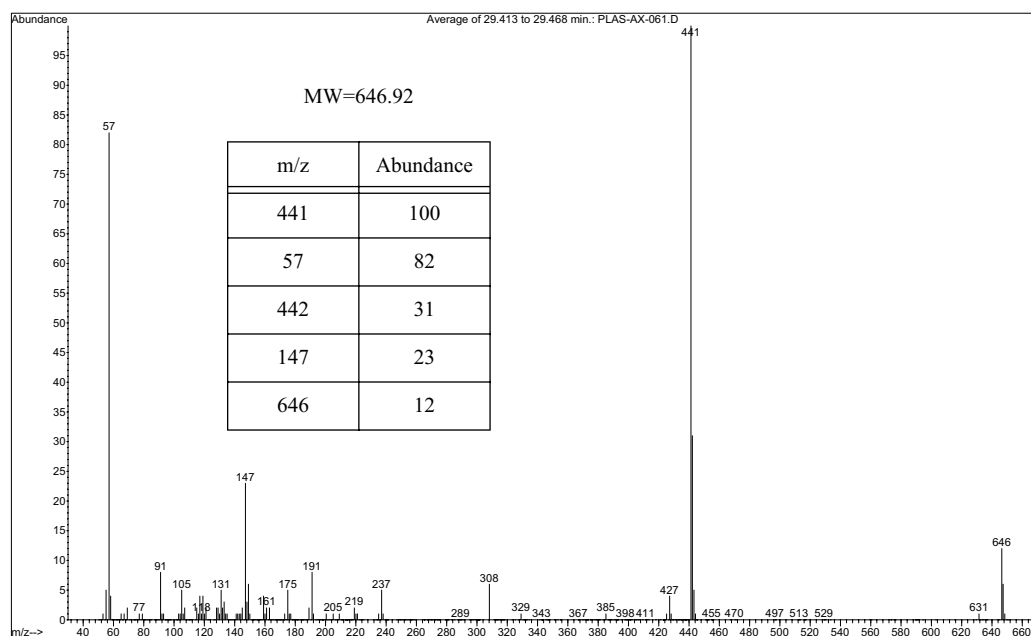
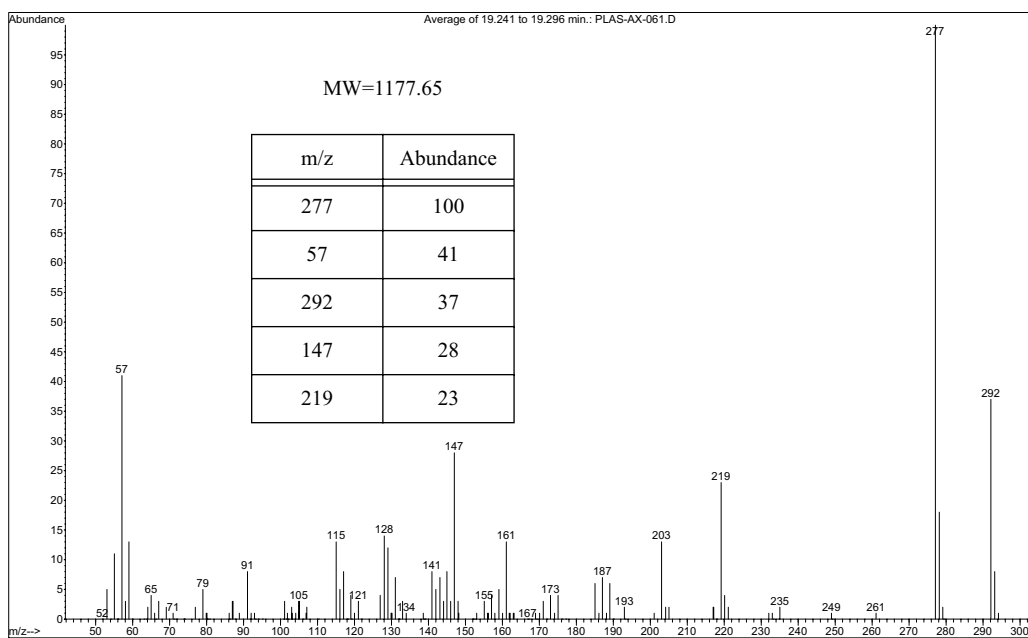
Experimental data shows that this category of chemicals is not readily biodegradable. This class of compounds photodegrades rapidly. In the environment, occurrence would be partitioned primarily to soil and sediments rather than air or water.

Point of Release

Migration is greater from polypropylene than from high-density polyethylene. Little migration is found to aqueous media. Migration is highest into n-heptane, ethanol, and corn oil.

Toxicological Data

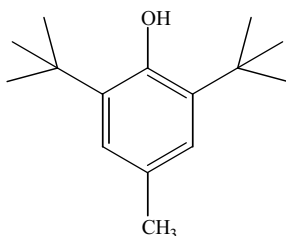
Toxicity of this compound is considered low. LD50 was not quantitated, rats tolerated administration of 5.0 g/kg body weight and mice tolerated up to 10 mg/kg body weight. Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectra for Naugard® B-25 - PLAS-AX-061

For Chromatogram See Appendix A - PLAS-AX-061 - page 505

Naugard® BHT

Chemtura Corporation

**CAS Number** 128-37-0**RTECS Number** GO7875000**Abbreviation** BHT**Formula** C₁₅H₂₄O**Molecular Weight** 220.35**Chemical Name**

2,6-di-tert-butyl-4-methylphenol

Synonyms

butylated hydroxytoluene; BHT; 2,6-di-tert-butyl-p-cresol

Brand Names & Manufacturers

Vulkanox® KB

Lanxess

Physical Properties**Appearance** White powder or granules**Melting Point** 69-71 °C**Boiling Point** 265 °C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 20-40	EtOH 26	Acetone U	CH₂Cl₂ U	Hexane U
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Application**Application, Regulatory & Environmental Information**

General purpose phenolic antioxidant used for polyolefin applications such as petroleum, animal feed, and for food products and packaging.

Regulatory Information

FDA approved for food contact. Approved under 21CFR175.105 – adhesives (no limitations), 175.125 – pressure sensitive adhesives (0.1% max.) and 177.2600 – rubber articles intended for repeated use (5% max.).

Environmental Impact

The substance is harmful to aquatic organisms. Log Pow value of 5.1 indicates a medium to high potential for this substance to bioaccumulate. If released into the environment, the main target compartment would be air.

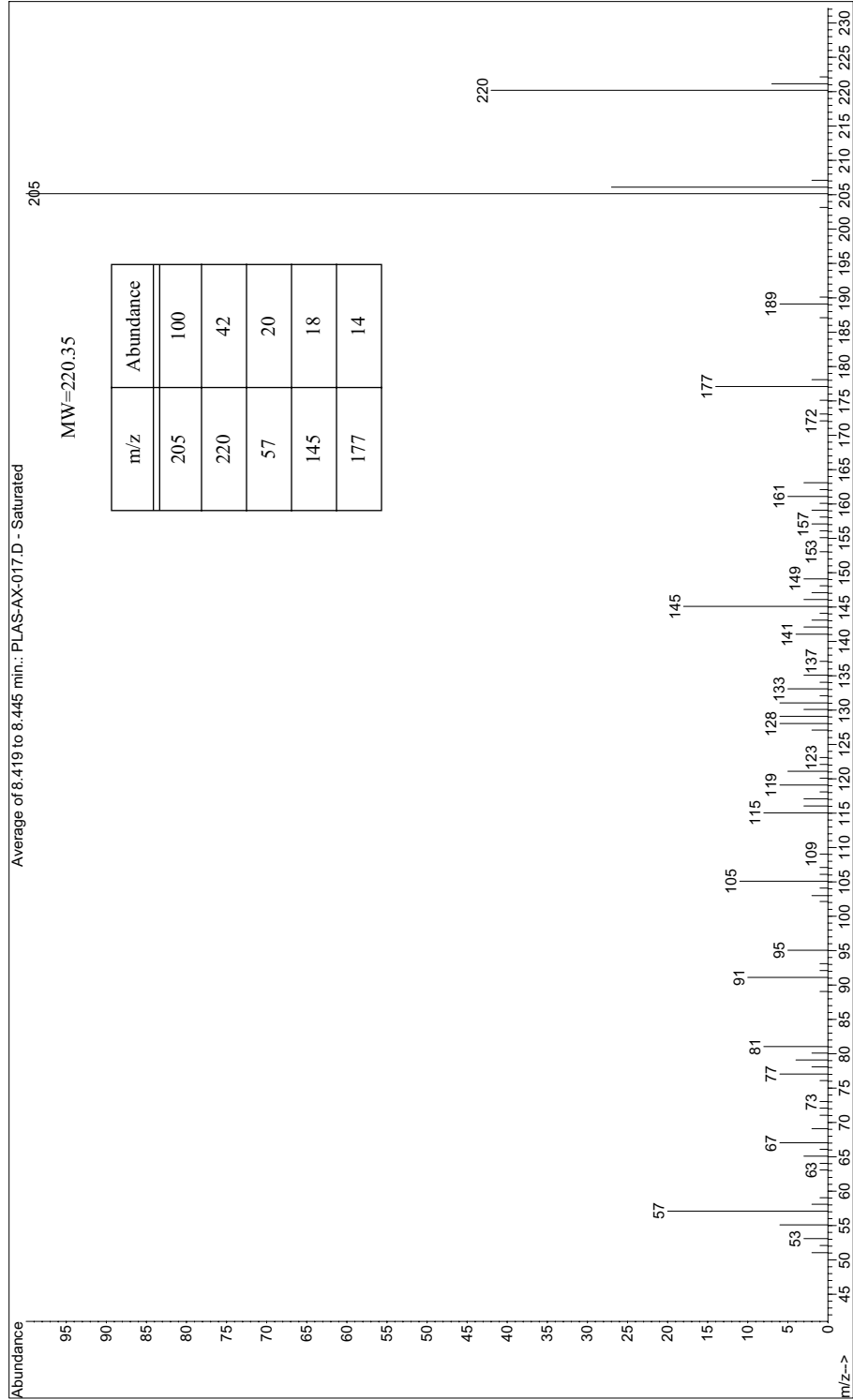
Point of Release

Releases into the environment may occur during production of BHT as well as during its use in different applications as stabilizer and during the use of the products that contain the substance. A significant release into the environment is expected from migration of BHT onto the surface of products containing the substance.

Toxicological Data

Oral (LD50): 890 mg/kg [Rat]. May have harmful effects on the liver.

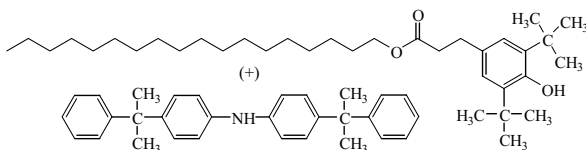
Mass Spectrum for Naugard® BHT - PLAS-AX-017



For Chromatogram See Appendix A - PLAS-AX-017 - page 506

Naugard® HM-22

Chemtura Corporation

**CAS Number** N/A**RTECS Number** N/A**Abbreviation** Not Identified**Formula** N/A**Molecular Weight** 531/406**Chemical Name**

blend of phenolic primary and diphenylamine secondary antioxidants (Naugards 76 and 445)

Synonyms

N/A

Brand Names & Manufacturers

Naugard HM-22

Chemtura Corporation

Physical Properties**Appearance** White granules**Melting Point** 49 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<1	U	80	U	<2

Application**Application, Regulatory & Environmental Information**

Naugard® HM-22 is a 1:1 granular blend of Naugard® 76 and Naugard® 445. This phenolic/amine blend provides synergistic short- and long-term thermal protection against oxidation in polypropylene. It also exhibits color and viscosity stability, as well as gelation and skinning resistance in SIS, SBS, EVA, PE, and polyamide hot melt adhesives.

Regulatory Information

This material is not FDA approved for food contact.

Environmental Impact

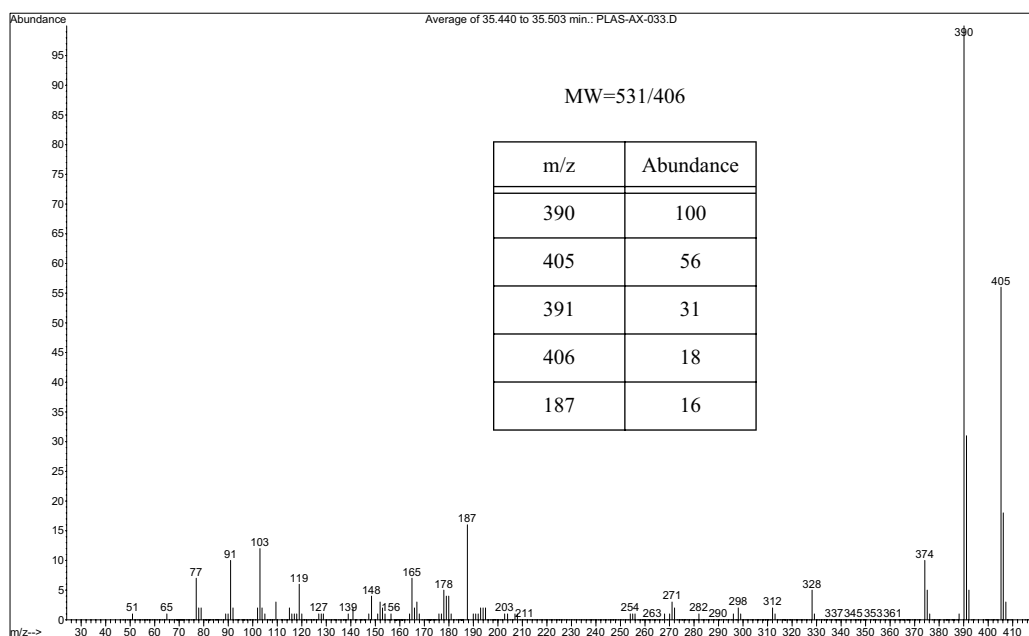
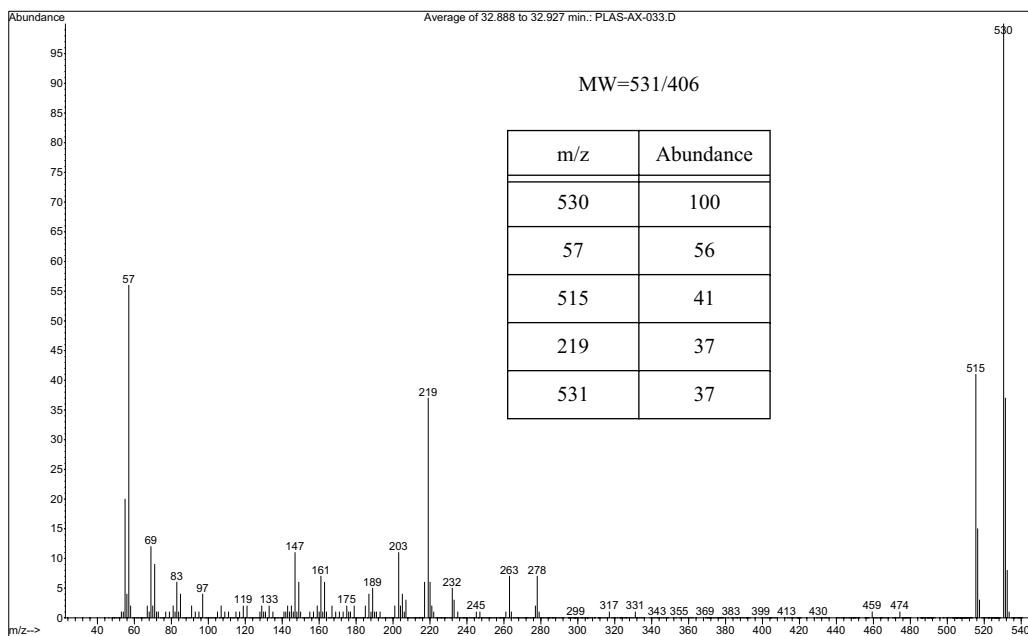
This material is not readily biodegradable. Log Pow value of ~8 indicates a high potential to bioaccumulate.

Point of Release

Can be released as a point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the longevity of the products and upon disposal of the products.

Toxicological Data

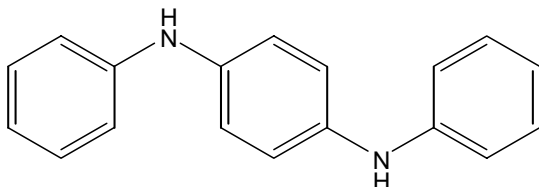
Acute toxicity: (LD50): >10000 mg/kg [Rat]. This material was not mutagenic in an Ames bacterial assay.

Mass Spectra for Naugard® HM-22 - PLAS-AX-033

For Chromatogram See Appendix A - PLAS-AX-033 - page 507

Naugard® J

Chemtura Corporation

**CAS Number** 74-31-7**RTECS Number** ST2275000**Abbreviation** DPPD**Formula** C₁₈H₁₆N₂**Molecular Weight** 260.36**Chemical Name**

N,N'-diphenyl-p-phenylenediamine

Synonyms

4-phenylaminodiphenylamine

Brand Names & Manufacturers

Agerite® DPPD

R.T. Vanderbilt

Physical Properties**Appearance** Light gray to brown powder**Melting Point** 144 °C**Boiling Point** 220-225 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	1-10	1-10	1-10

Application**Application, Regulatory & Environmental Information**

Amine antioxidant that offers protection against degradation due to copper and manganese. It also offers protection against outdoor flexing and static weather cracking in natural rubber and against thermal oxidation in polyethylene. Inhibits gum formation and degradation at elevated temperature in petroleum oils.

Regulatory Information

No information available.

Environmental Impact

Harmful to the environment. May cause long-term adverse effects.

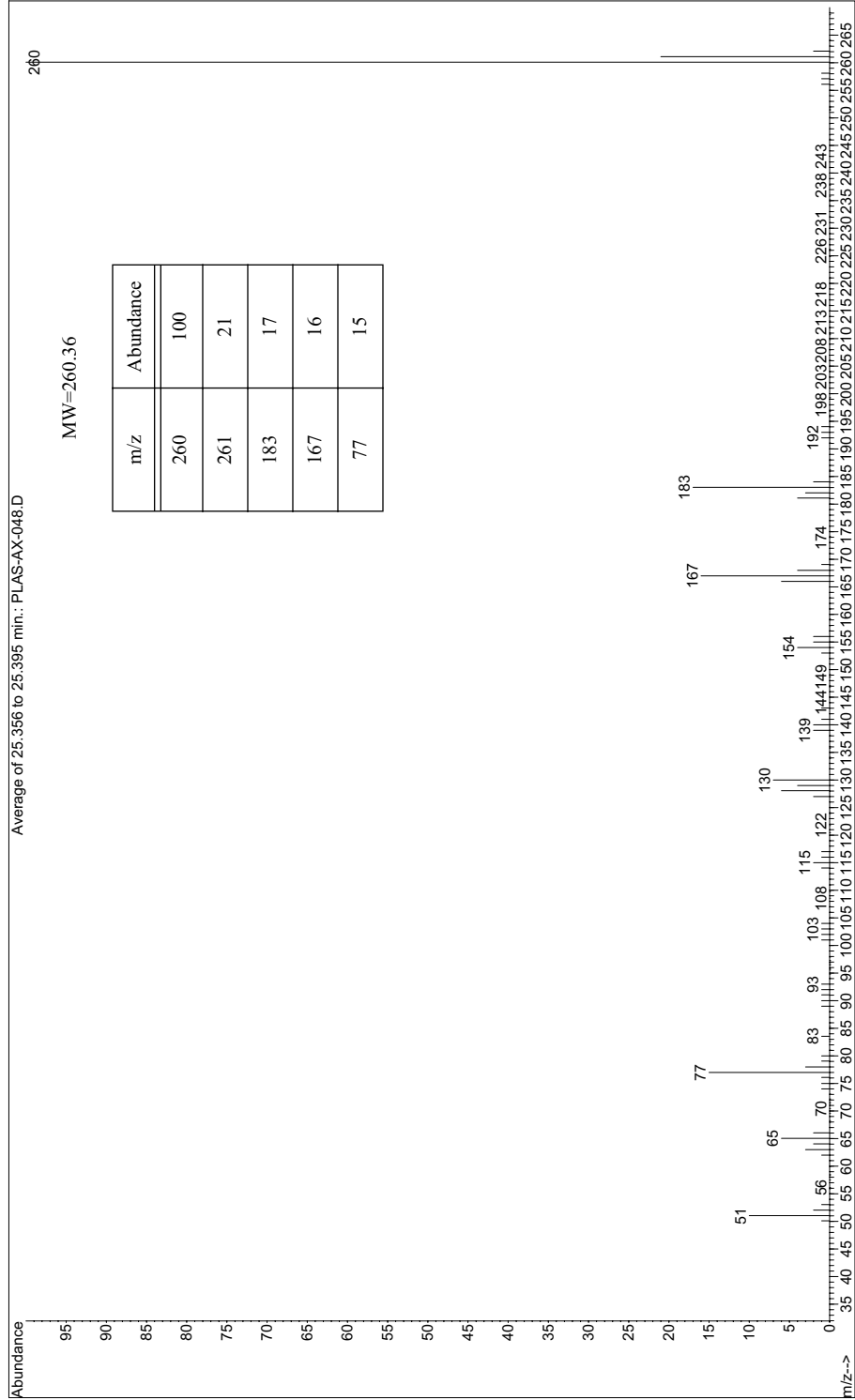
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): 2370 mg/kg [Rat]. Suspected developmental toxin.

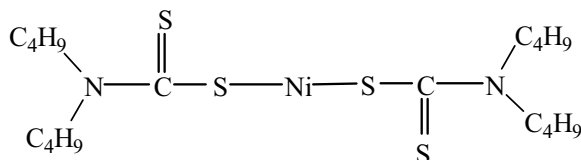
Mass Spectrum for Naugard® J - PLAS-AX-048



For Chromatogram See Appendix A - PLAS-AX-048 - page 508

Naugard® NBC

Chemtura Corporation



CAS Number 13927-77-0

RTECS Number QR6140000

Abbreviation NBC

Formula $C_{18}H_{36}N_2NiS_4$

Molecular Weight 467.45

Chemical Name

nickel dibutyl dithiocarbamate

Synonyms

di-N-butyl dithiocarbamic acid, nickel salt; nickel N,N-di-n-dibutyl dithiocarbamate; nickel dibutyl dithiocarbamate

Brand Names & Manufacturers

Antiozonant NIBUD

Akrochem Corporation

Nocrac™ NBC

Ohuchi Shinko Co., Ltd.

Perkacit® NDBC

Akzo Nobel Chemicals B.V.

Physical Properties**Appearance** Green powder**Melting Point** 85 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	40-80	40-80	U

Application**Application, Regulatory & Environmental Information**

Used as a secondary accelerator with antioxidant, antiozonant, and stabilizing function in synthetic rubber and high polymer materials in the plastics and rubber industries. Mainly used in styrene-butadiene rubber (SBR), chloroprene rubber (CR), epichlorohydrin, and chlorosulfonated polyethylene rubber. Promotes heat-resistance of chlorosulfonated polyethylene rubber, EPDM and CSM, and sunshine resistance of CR.

Regulatory Information

This product is regulated for use in articles in contact with food as specified under BgVV XXI, Category 4 at 0.3 to 0.5%. It does not have FDA approval for food contact applications.

Environmental Impact

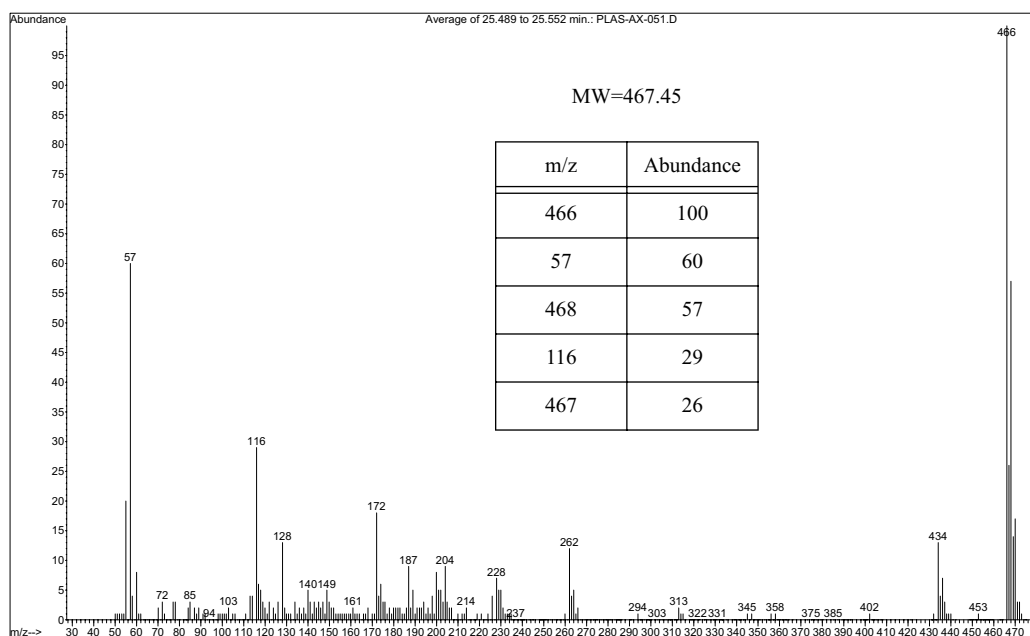
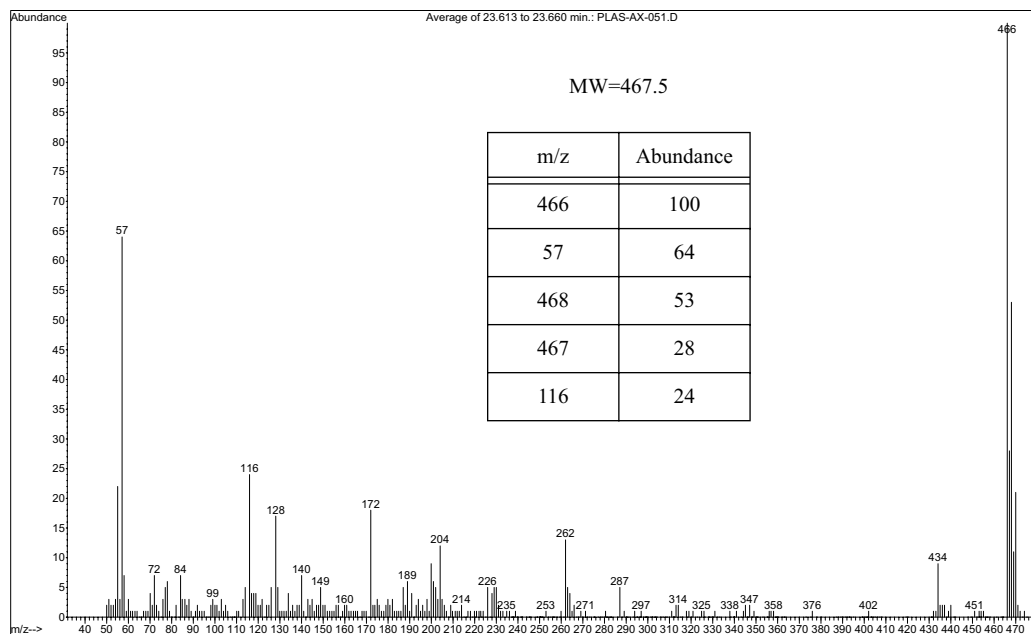
Ecological impact not determined. Similar compounds show low to moderate biodegradability, but rapid hydrolysis under acidic conditions. Similar compounds are also determined to have low bioaccumulation potential and environmental persistence. Bioconcentration factor (BCF) is 307.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

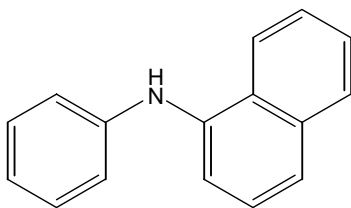
Classified as a confirmed carcinogen by RTECS and ACGIH, and "anticipated human carcinogen" by the NTP. (LD50): 17 g/kg BW [Rat]. Induced lung cancer in mice after 1.5 years exposure.

Mass Spectrum for Naugard® NBC - PLAS-AX-051

For Chromatogram See Appendix A - PLAS-AX-051 - page 509

Naugard® PANA

Chemtura Corporation

**CAS Number** 90-30-2**RTECS Number** QM4500000**Abbreviation** PNA-1**Formula** C₁₆H₁₃N**Molecular Weight** 219.28**Chemical Name**

N-phenyl-1-naphthylamine

Synonyms

1-anilinonaphthalene; phenyl-alpha-naphthylamine

Brand Names & Manufacturers

Antioxidant PANA

Akrochem Corporation

Vulkanox® PAN

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** Light brown to violet crystalline powder**Melting Point** 55 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Used as a general purpose antioxidant for CR, NR, and SBR. Can be used as a gel inhibitor.

Regulatory Information

FDA approved for food contact under 21CFR177.2600 – rubber articles intended for repeat uses, not to exceed 5% by weight of the total composition and 21CFR178.3570 – lubricants with incidental food contact not to exceed 1% by weight of the total composition.

Environmental Impact

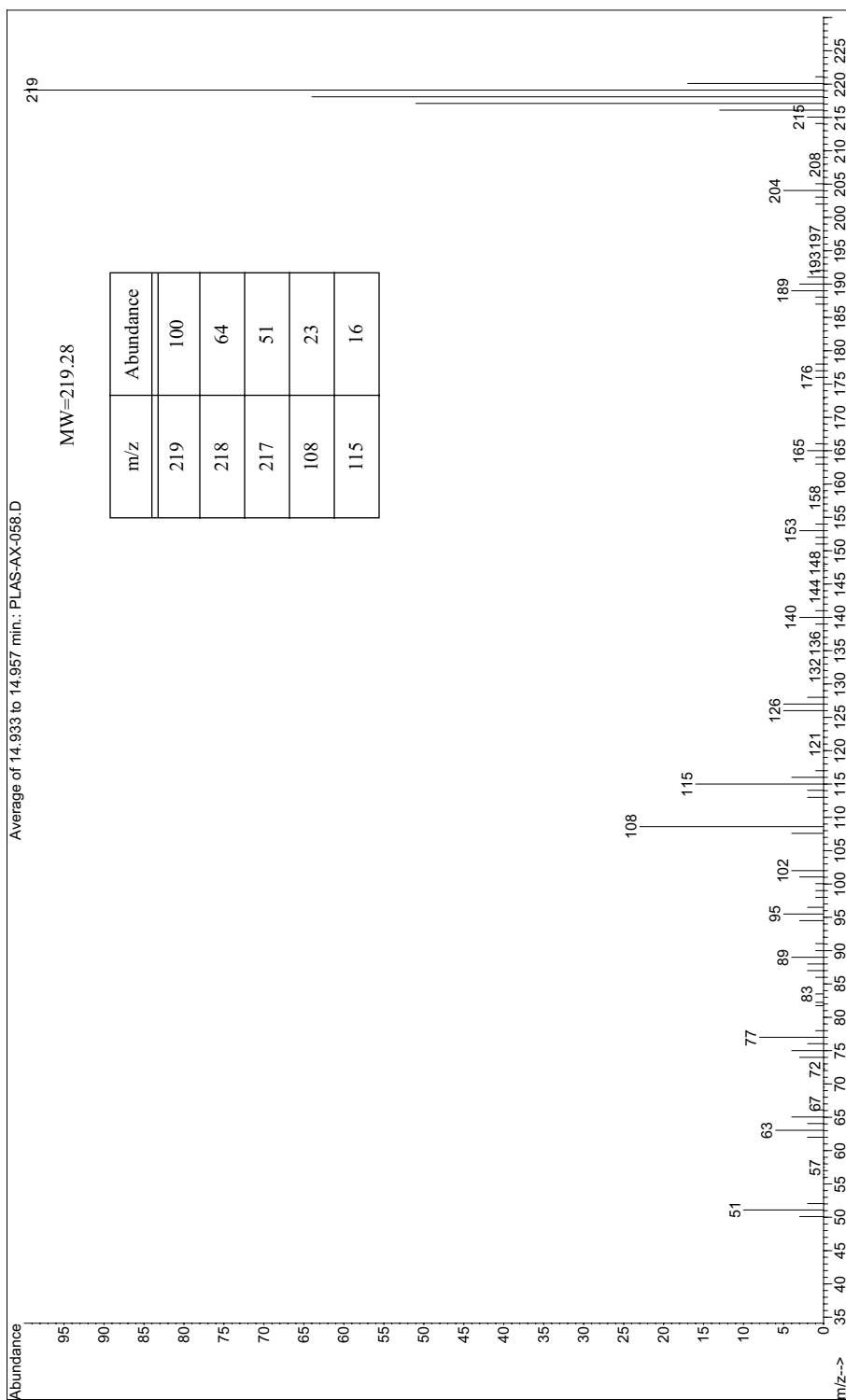
This substance is very toxic to aquatic organisms. The reported log Pow value is 4.2, indicating a moderate potential to bioaccumulate.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

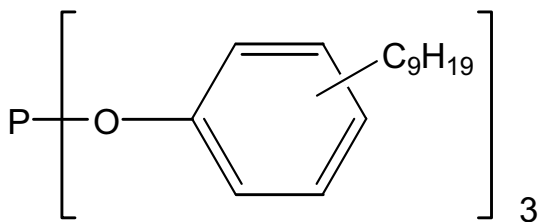
Acute oral (LD50): 1630 mg/kg [Rat]. Experimental evidence suggests carcinogenic potential.

Mass Spectrum for Naugard® PANA - PLAS-AX-058

For Chromatogram See Appendix A - PLAS-AX-058 - page 510

Naugard® PHR

Chemtura Corporation



CAS Number 26523-78-4

RTECS Number N/A

Abbreviation TNPP

Formula $C_{45}H_{69}O_3P$

Molecular Weight 689.32

Chemical Name

tris(monononylphenyl) phosphite with up to 1% triisopropanol amine

Synonyms

nonylphenyl phosphite (3:1); tris(monononylphenyl) phosphite; tris nonylphenyl phosphite; tris(monononylphenyl)phosphite, 2,2'-methylenebis(4-methyl-6-nonylphenol)

Brand Names & Manufacturers

Naugard PHR

Chemtura Corporation

Physical Properties**Appearance** Light yellow viscous liquid**Melting Point** Not available**Boiling Point** >360 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<2.3	U	100	U	100

Application, Regulatory & Environmental Information**Application**

Secondary liquid phosphite antioxidant that functions as a peroxide decomposer and as a processing stabilizer in a wide variety of polymers, including polyolefins and styrenics.

Regulatory Information

FDA approved under 21CFR175.125 – pressure sensitive adhesives; 175.300 – resinous and polymeric coatings; 175.390 – zinc-silicon dioxide matrix coatings; 177.1210 – closures with sealing gaskets for food containers; 177.2600 – rubber articles intended for repeated use, and 178.2010 – antioxidants and/or stabilizers for polymers.

Environmental Impact

Classified as an environmentally hazardous substance and considered to be a marine pollutant.

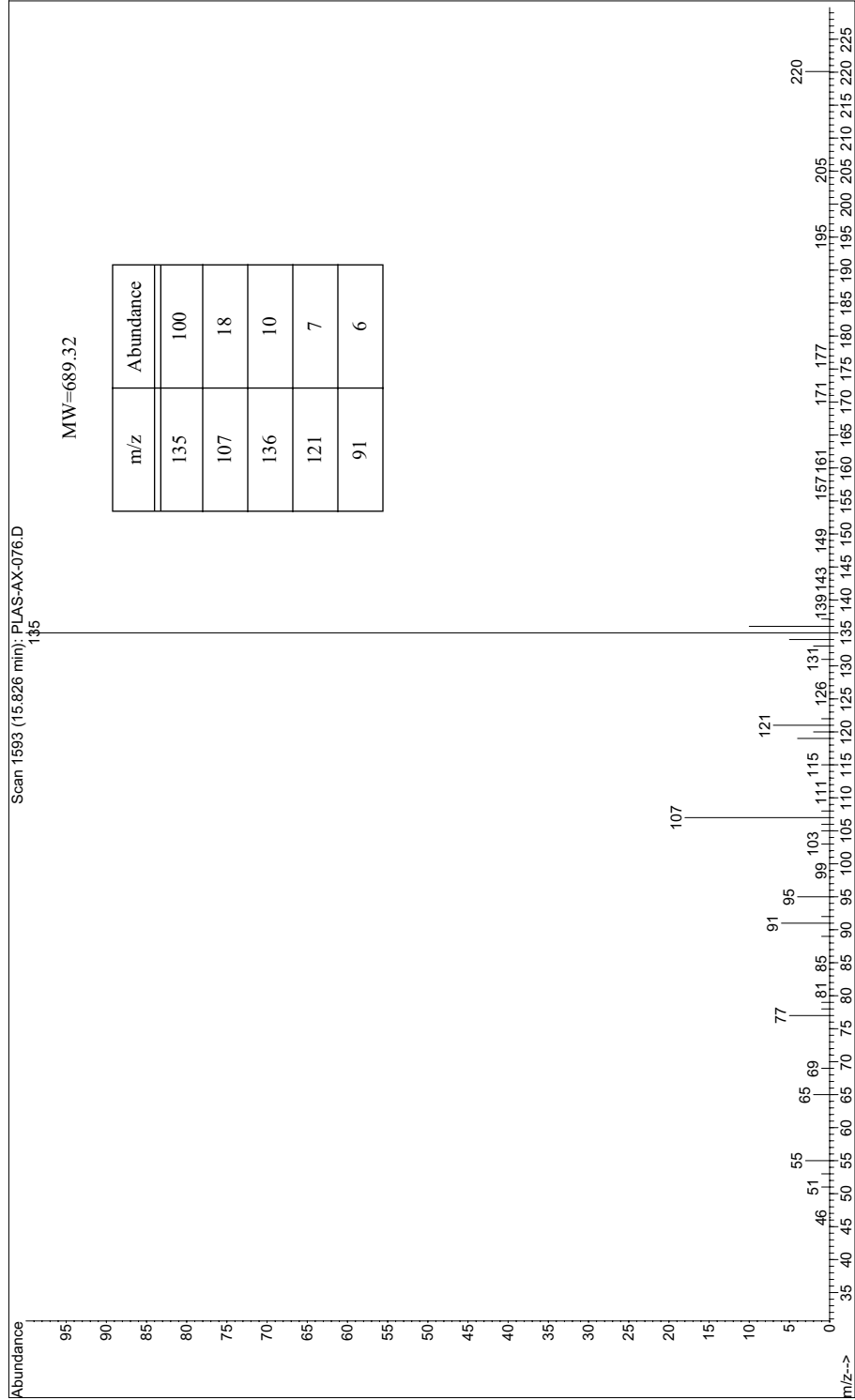
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

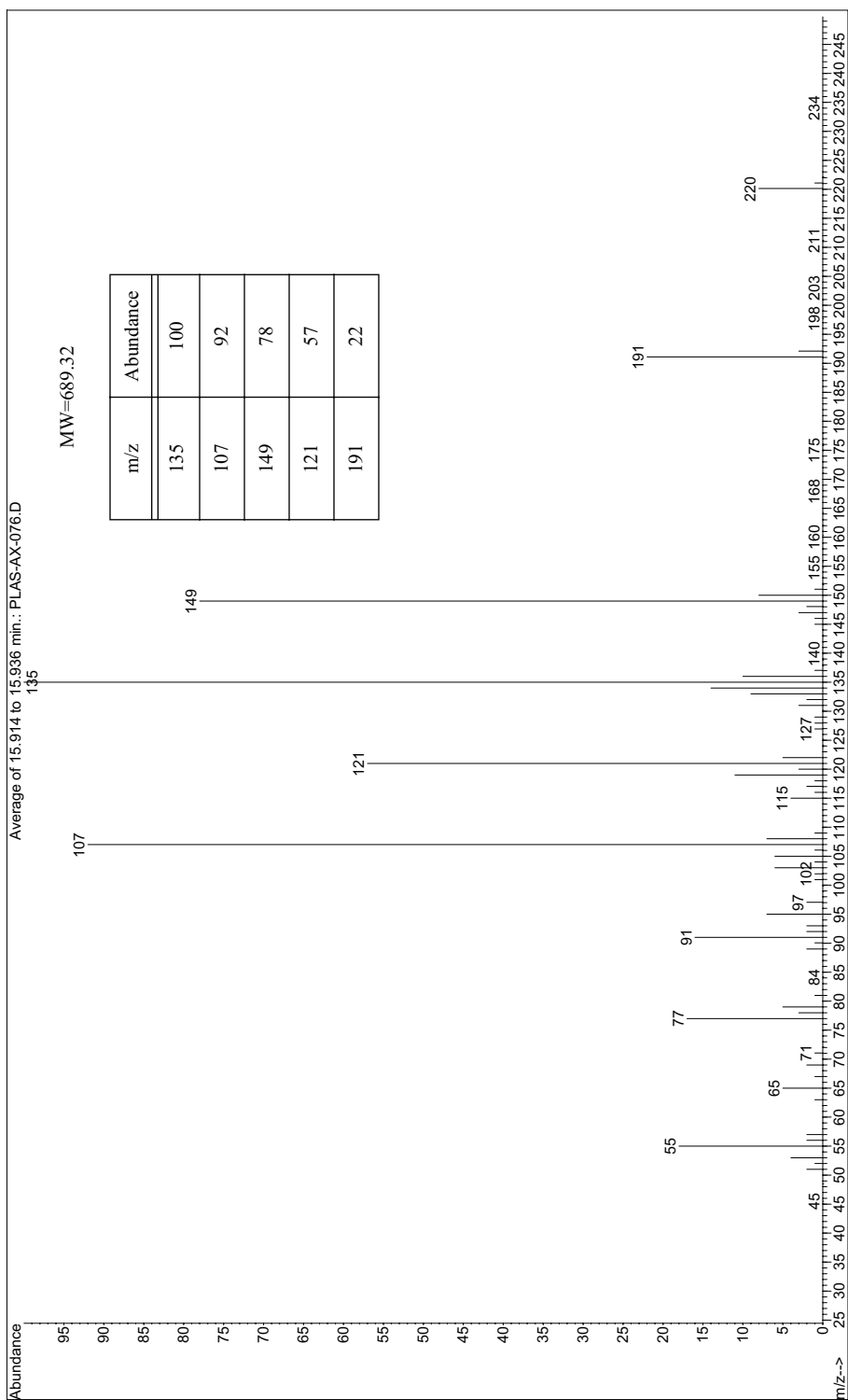
Toxicological Data

Oral (LD50): >2000 mg/kg [Rat]; skin (LD50): > 2000 mg/kg [Rabbit]. Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectrum for Naugard® PHR - PLAS-AX-076

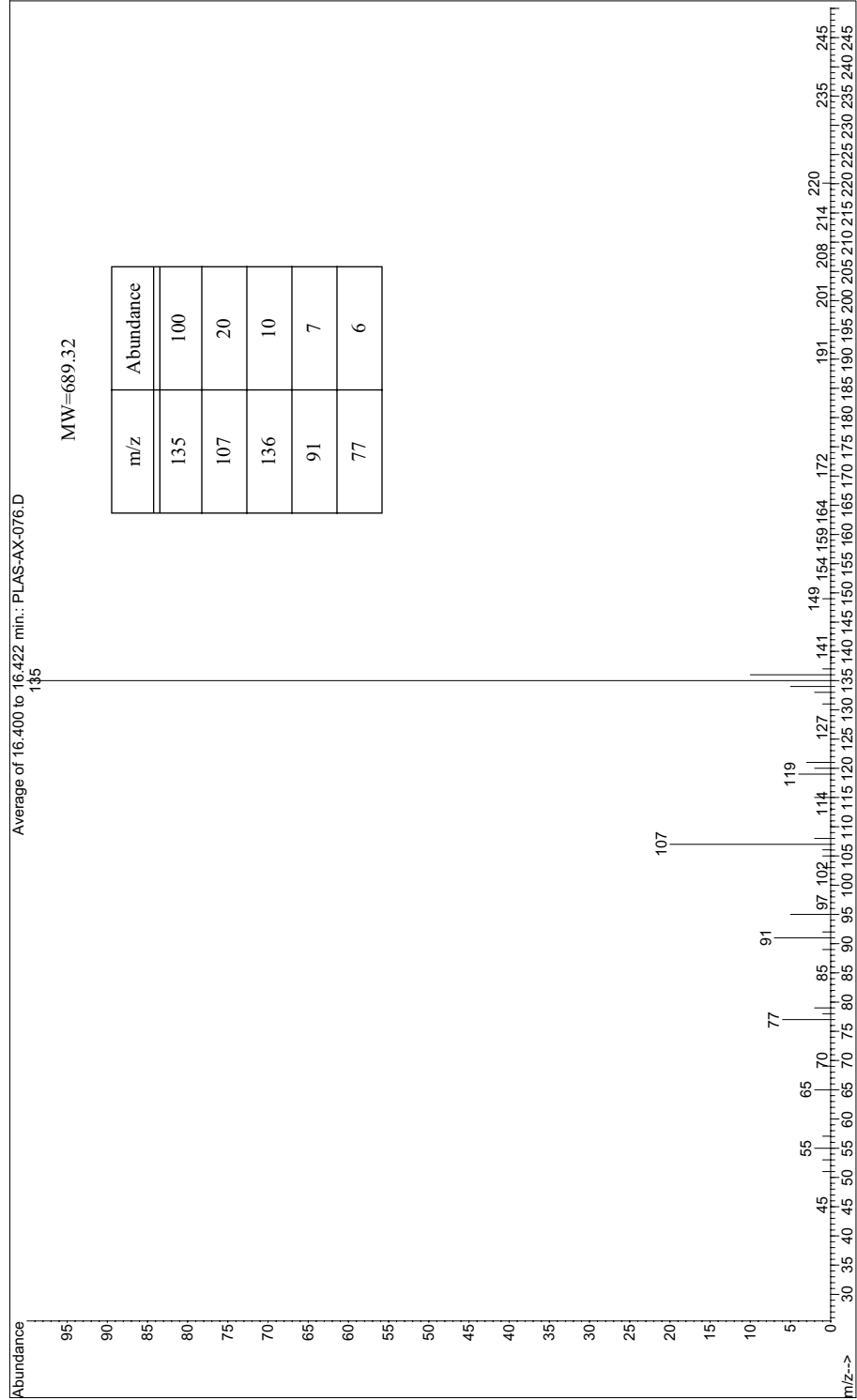


For Chromatogram See Appendix A - PLAS-AX-076 - page 511

Mass Spectrum for Naugard® PHR - PLAS-AX-076

For Chromatogram See Appendix A - PLAS-AX-076 - page 511

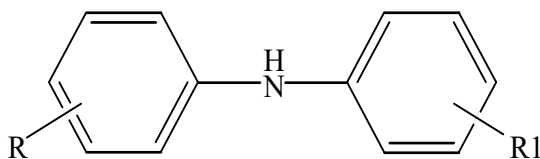
Mass Spectrum for Naugard® PHR - PLAS-AX-076



For Chromatogram See Appendix A - PLAS-AX-076 - page 511

Naugard® PS-30

Chemtura Corporation

**CAS Number** 68411-46-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₁₂H₁₁N • C₈H₁₆**Molecular Weight** 281 (typical)**Chemical Name**

benzenamine, N-phenyl, reaction products with 2,4,4-trimethylpentene

Synonyms

diphenylamine, diisobutylene reaction product; N-phenylbenzenamine, 2,4,4-trimethyl-1-pentene, and 2,4,4-trimethyl-2-pentene reaction product; octylated diphenylamine

Brand Names & Manufacturers

Antioxidant S	Akrochem Corporation
Stangard® ODP	Harwick Chemical Corporation
Stalite® S	B.F. Goodrich Company
Vanox® 12	R.T. Vanderbilt Company, Inc.

Physical Properties**Appearance** Clear reddish to brown liquid**Melting Point** N/A**Boiling Point** >200°C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	10-40	10-40	10-40

Application, Regulatory & Environmental Information**Application**

Naugard® PS-30 is a liquid amine antioxidant typically combined with phenolic antioxidants, phosphites, and synergists in polyether polyols to inhibit physical/color scorch associated with the production of flexible urethane foam.

Regulatory Information

FDA approved 2001 for use as an antioxidant with 2,4,4-trimethylpentene (at levels not to exceed 0.5 % weight of lubricant), in lubricants used in machinery (with incidental food contact) in production, manufacturing, packing, processing, preparing, treating, packaging, transporting, or storage applications, 21CFR 178.3570.

Environmental Impact

Possibly hazardous short-term degradation products are not likely. However, long-term degradation products may arise.

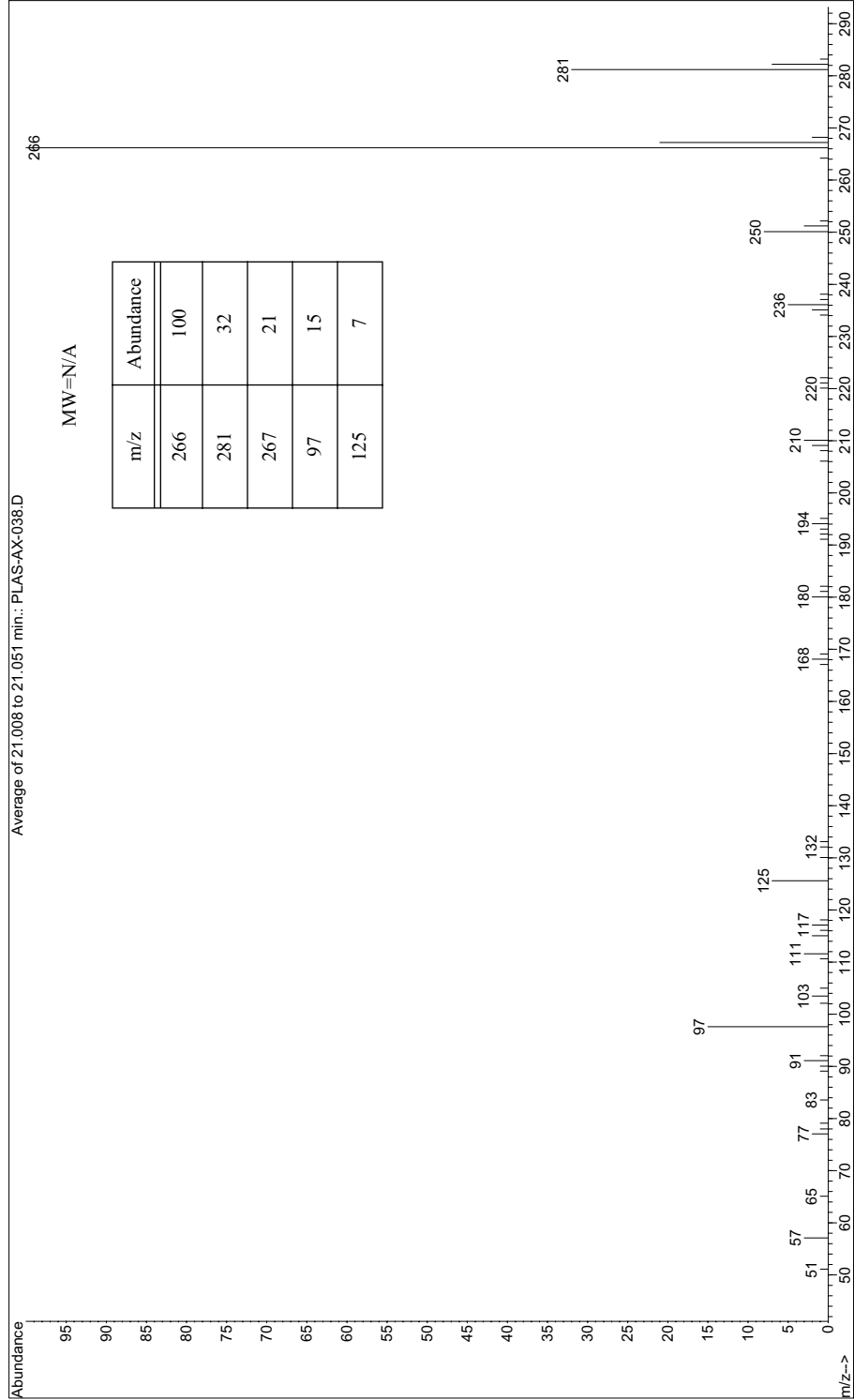
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

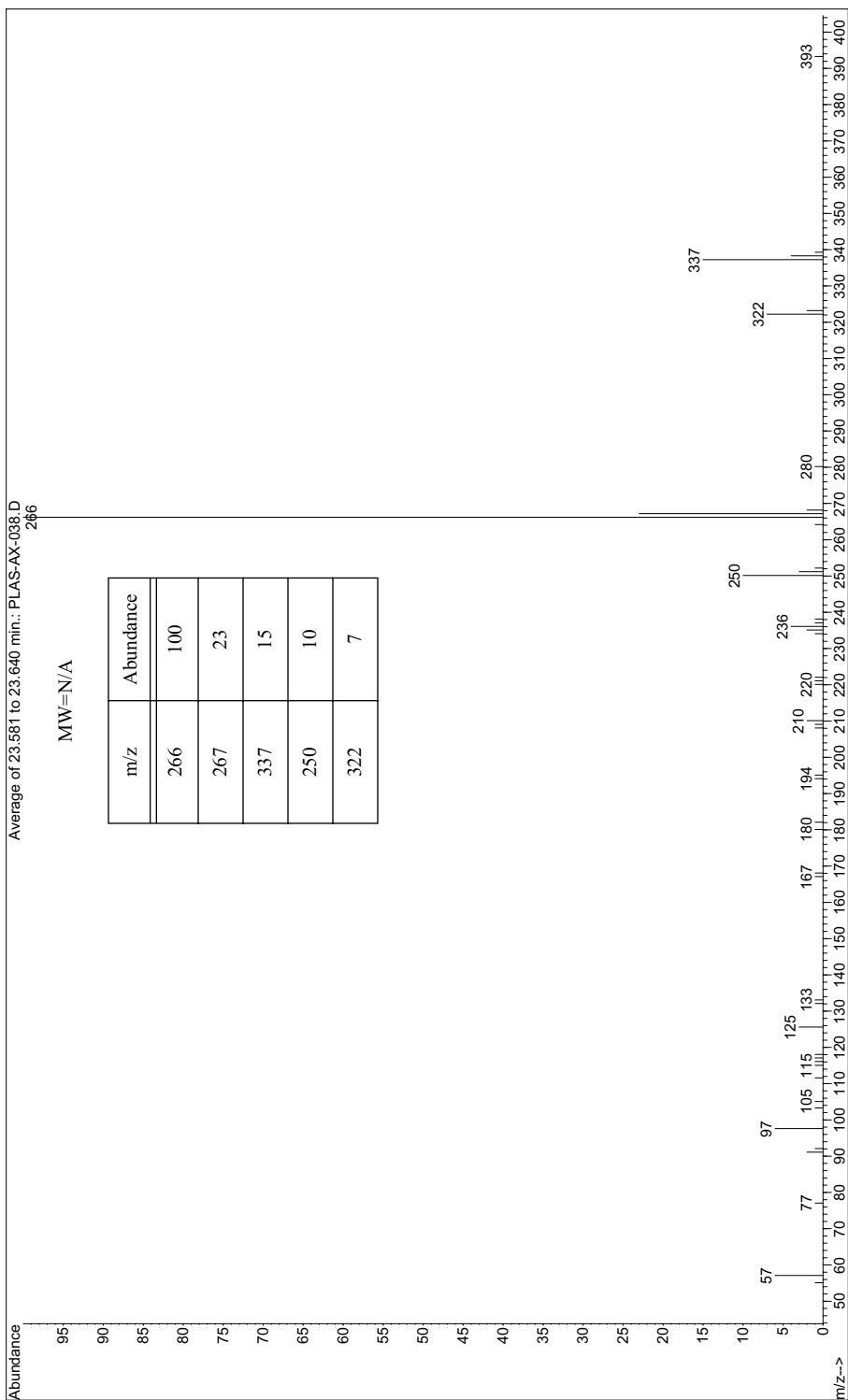
Toxicological Data

High levels of this material in the diet caused degenerative changes in the liver, kidney, adrenal medulla, and thyroid of rats and a decrease of blood prothrombin content in rats and dogs. Mutagenicity: This material was not mutagenic in an Ames bacterial assay. Acute oral toxicity (LD50): 7580 mg/kg [Rat].

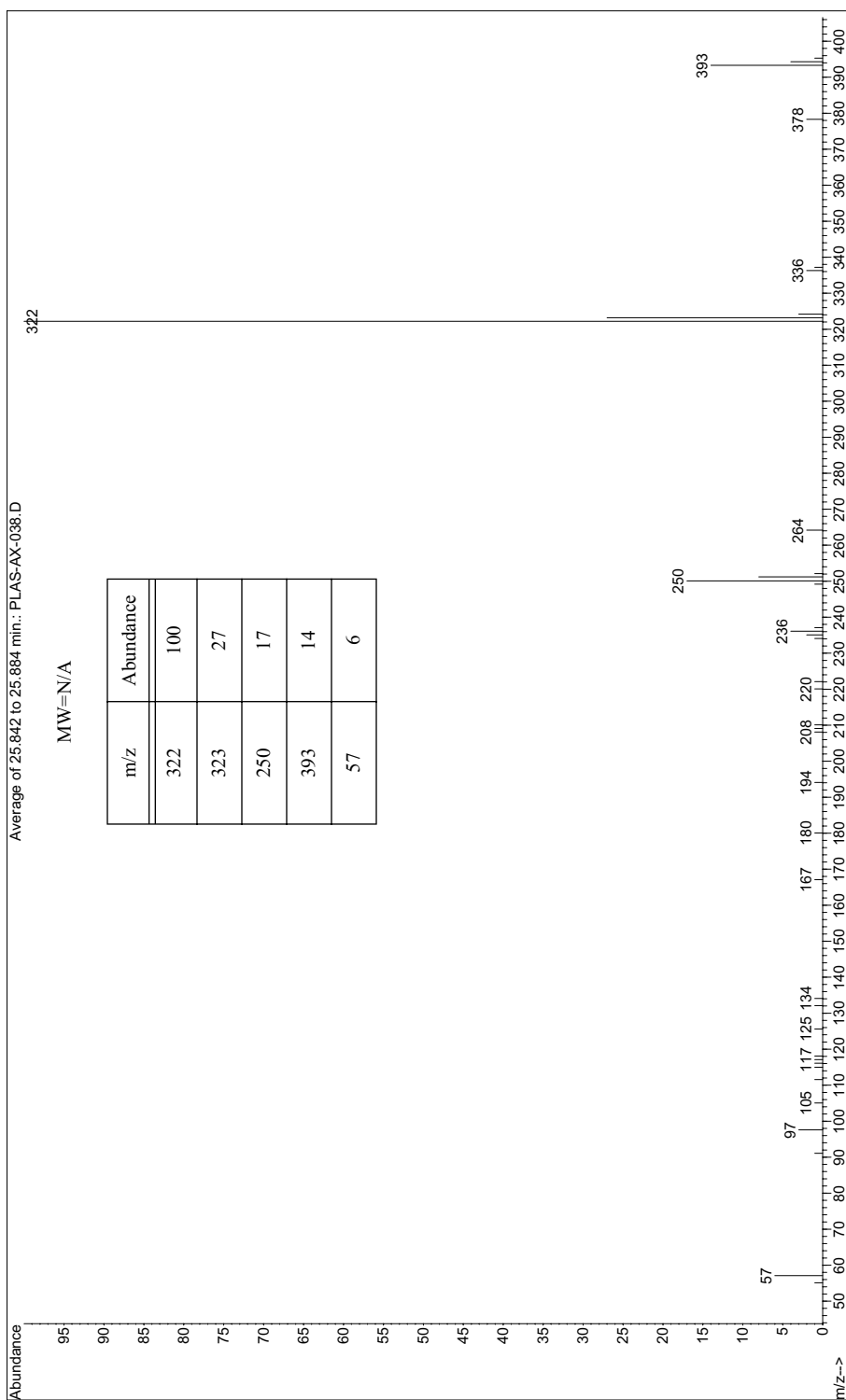
Mass Spectrum for Naugard® PS-30 - PLAS-AX-038



For Chromatogram See Appendix A - PLAS-AX-038 - page 512

Mass Spectrum for Naugard® PS-30 - PLAS-AX-038

For Chromatogram See Appendix A - PLAS-AX-038 - page 512

Mass Spectrum for Naugard® PS-30 - PLAS-AX-038

For Chromatogram See Appendix A - PLAS-AX-038 - page 512

Naugard® PS-35

Chemtura Corporation

Unspecified Structure

CAS Number N/A

RTECS Number N/A

Abbreviation Not Identified

Formula N/A

Molecular Weight N/A

Chemical Name

ternary blend of phenol, phosphites, and amines

Synonyms

N/A

Brand Names & Manufacturers

Naugard PS-35

Chemtura Corporation

Physical Properties
Appearance Clear liquid**Melting Point** Not available**Boiling Point** 230 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	U	40-80	40-80	<0.1

Application**Application, Regulatory & Environmental Information**

An optimized blend of liquid phenolic antioxidant and liquid aromatic amine antioxidant with a small amount of a phosphite stabilizer. This blend was specifically developed for use as a heat and color stabilizer for polyols used for making flexible polyurethane foam.

Regulatory Information

No information available on FDA regulations regarding this specific blend, but several of the components are approved for indirect food contact per 21CFR175.105.

Environmental Impact

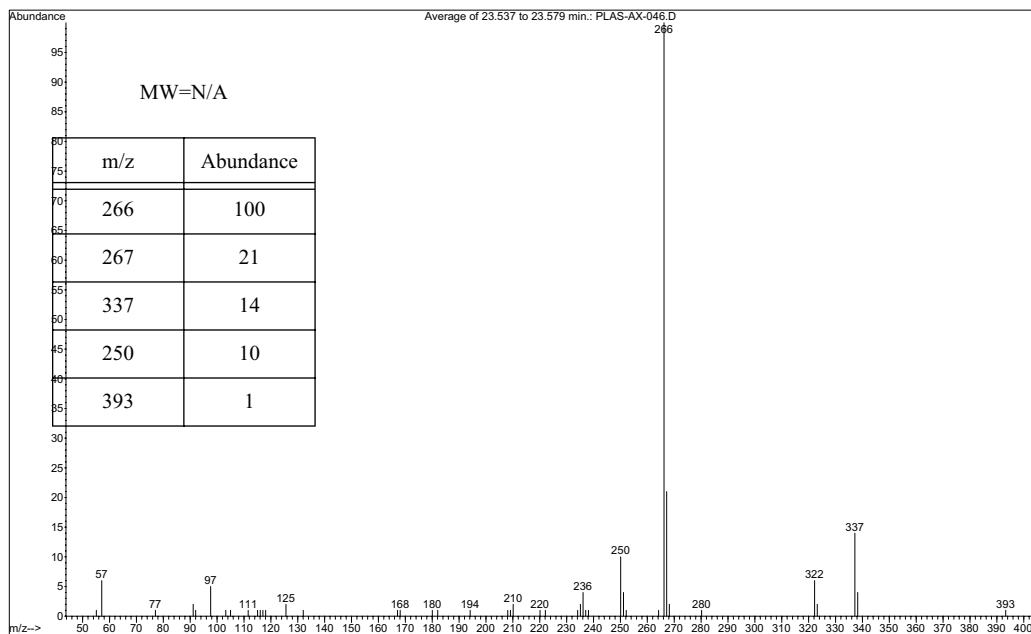
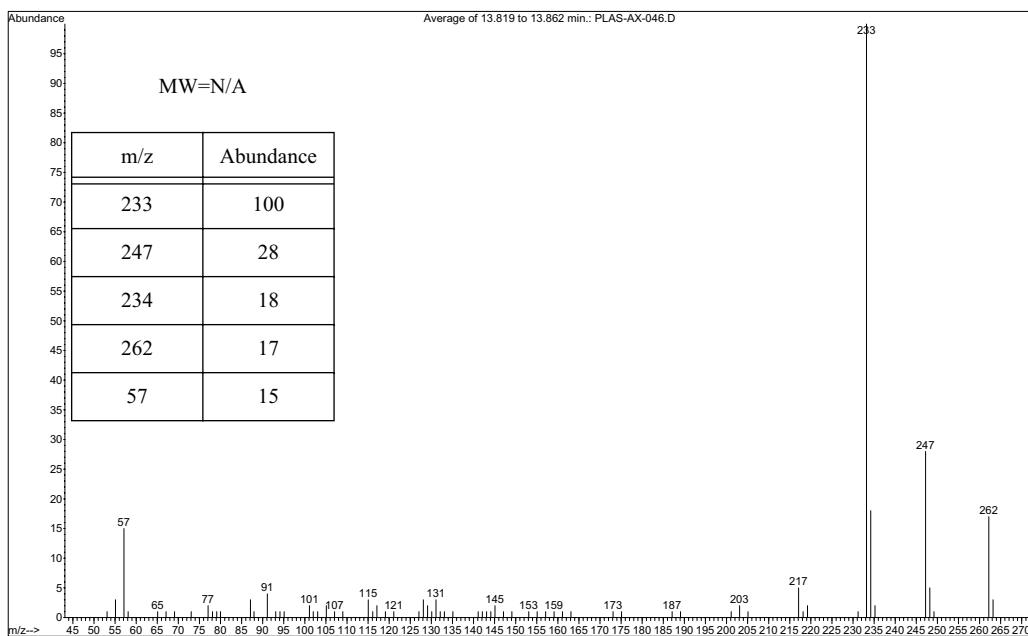
Based on data from the individual components of this blend, the log Kow value would be expected to be <4, indicating a low potential for bioaccumulation. Also, due to its insolubility in water, it is not likely to be toxic to aquatic wildlife.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

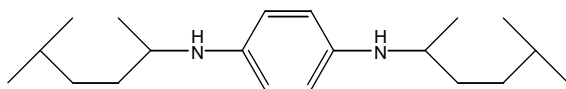
Acute oral toxicity (LD50): 1670 mg/kg [Rat]. Lowest published toxic oral dose (TDLo): 10914 mg/kg/3W-C [Rat].

Mass Spectra for Naugard® PS-35 - PLAS-AX-046

For Chromatogram See Appendix A - PLAS-AX-046 - page 513

Naugard® Q Extra

Chemtura Corporation

**CAS Number** 26780-96-1**RTECS Number** VB4900000**Abbreviation** DTQ**Formula** C₁₂H₁₅N**Molecular Weight** 173.25**Chemical Name**

1,2-dihydro-2,2,4-trimethylquinoline (polymerized)

Synonyms

2,2,4-trimethyl-1,2-dihydroquinone; acetonanyl

Brand Names & Manufacturers

Agerite® resin D

R.T. Vanderbilt Company, Inc.

Flectol® A

Flexsys America L.P.

Vulkanox® HS/LG

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** Reddish-brown drops**Melting Point** 85-120 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
<0.1		U	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Protects against thermo-oxidative degradation in natural and synthetic rubbers as well as plastics. It is commonly used in applications such as tire casings, wire breaker retreads, apex, belts, hoses, seals, mechanical goods, footwear, and wire.

Regulatory Information

Not FDA approved for food contact applications.

Environmental Impact

May be harmful to aquatic life and cause long-term adverse effects in the aquatic environment.

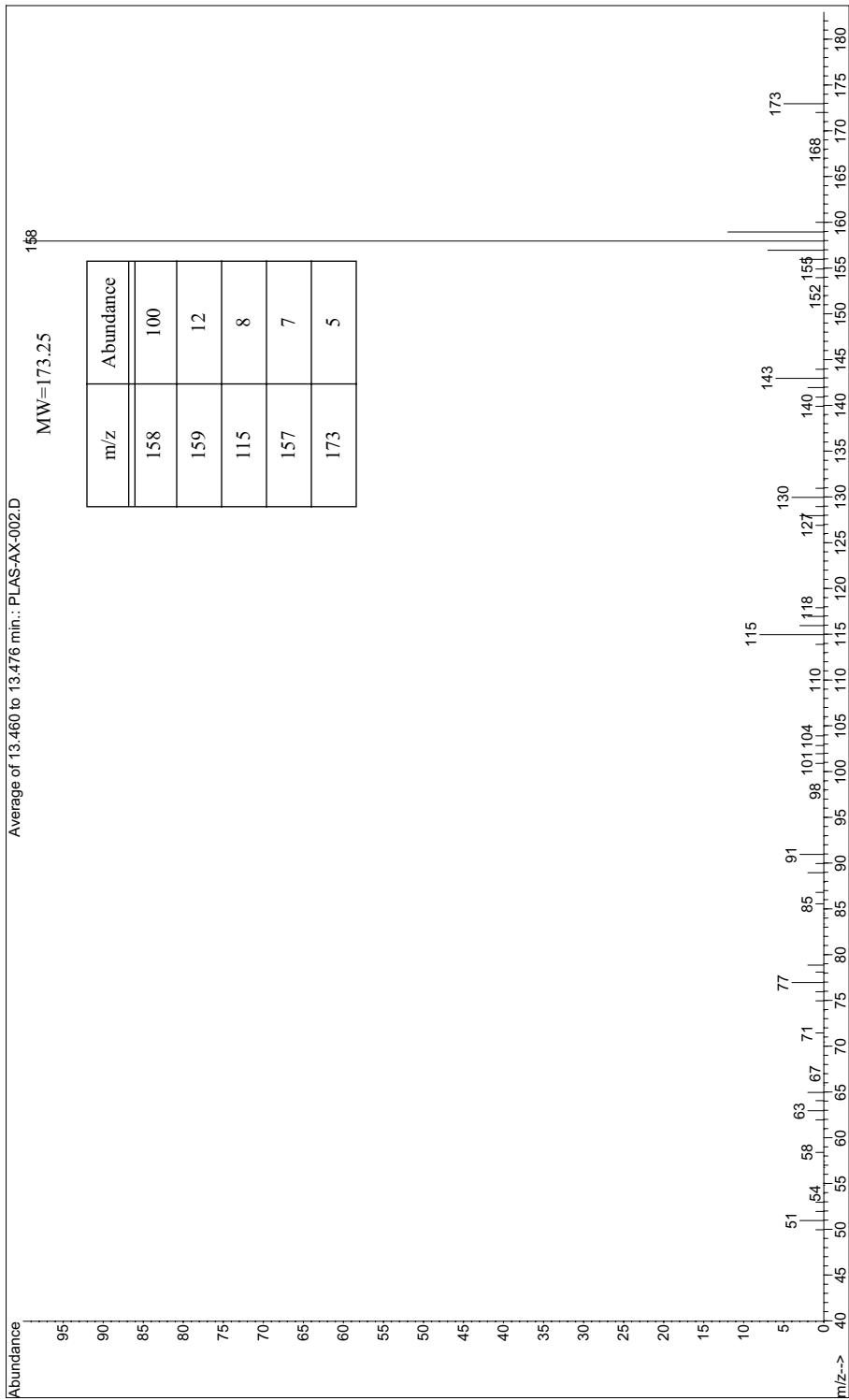
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

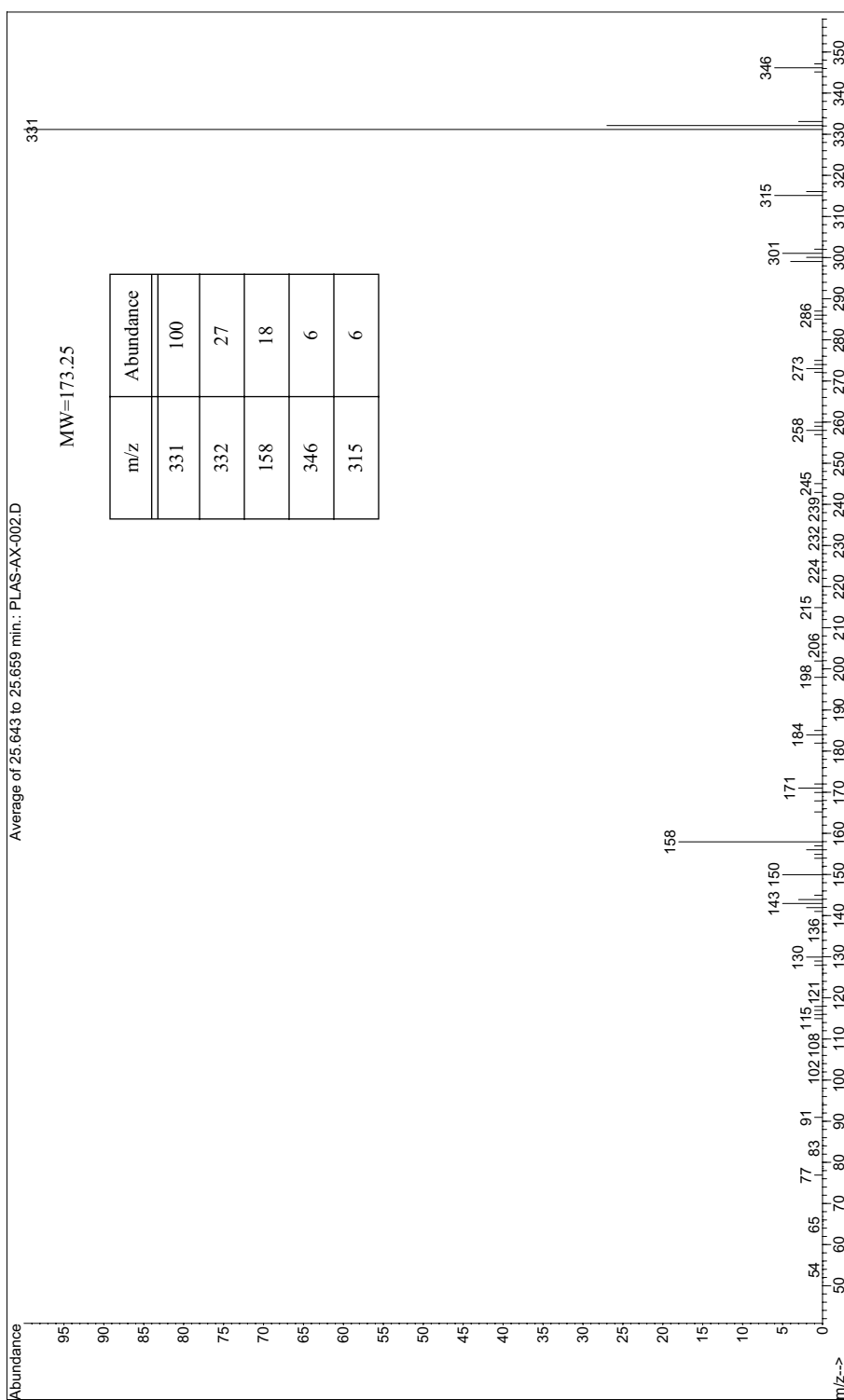
Toxicological Data

Poisonous doses target and inhibit CNS function; long-term toxicity also decreases BW gain, causes anemia, disrupts liver function in addition to CNS inhibition, decreases hemoglobin and erythrocytes. There is some evidence of carcinogenicity. Not determined to be mutagenic. (LD50): 2 g/kg BW oral [Rats and Rabbits], (LD50): 1.45 g/kg BW oral [Mouse].

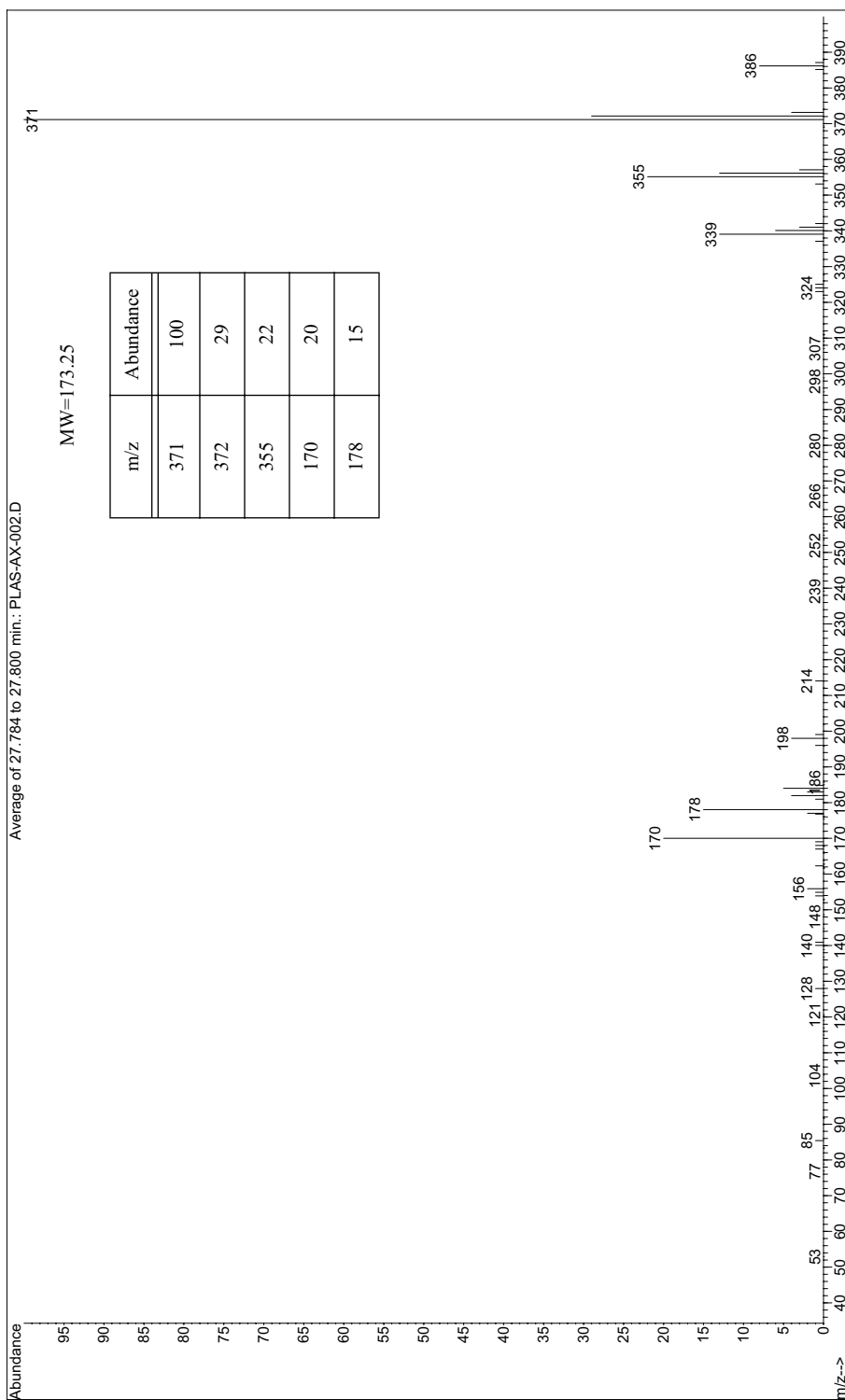
Mass Spectrum for Naugard® Q Extra - PLAS-AX-002



For Chromatogram See Appendix A - PLAS-AX-002 - page 514

Mass Spectrum for Naugard® Q Extra - PLAS-AX-002

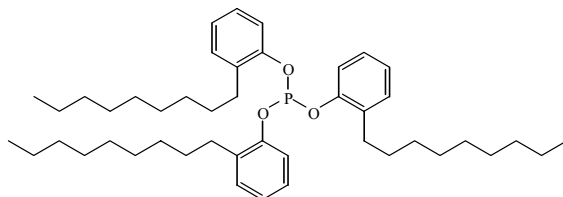
For Chromatogram See Appendix A - PLAS-AX-002 - page 514

Mass Spectrum for Naugard® Q Extra - PLAS-AX-002

For Chromatogram See Appendix A - PLAS-AX-002 - page 514

Naugard® RM-51

Chemtura Corporation

**CAS Number** 26523-78-4**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₄₅H₆₉O₃P**Molecular Weight** 689.00**Chemical Name**

blend of phenolic primary and phosphite secondary antioxidants

Synonyms

nonylphenyl phosphite (3:1); tris(mono-nonylphenyl) phosphite; tris nonylphenyl phosphite; tris(mono-nonylphenyl)phosphite, 2,2'-methylenebis(4-methyl-6-nonylphenol)

Brand Names & Manufacturers

Chemtura Corporation

Physical Properties**Appearance** Clear, gold to yellow viscous liquid**Melting Point** N/A**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	1-10	1-10	1-10

Application, Regulatory & Environmental Information**Application**

This material is an effective liquid antioxidant that is nonstaining and nondiscoloring. It is used in natural and synthetic rubbers for protection against oxygen, light, and heat.

Regulatory Information

FDA approval under 21CFR177.2600 – Rubber Articles Intended for Repeated Use – Limitation – 5% Max.

Environmental Impact

(EC50 48 hour): 0.42 mg/mL [Daphnia magna], (LC50 96 hour): < 10 mg/mL [Zebra fish]. (EBC50): > 100 mg/mL [Green algae], (LC50): > 100 mg/mL [Aerobic bacteria].

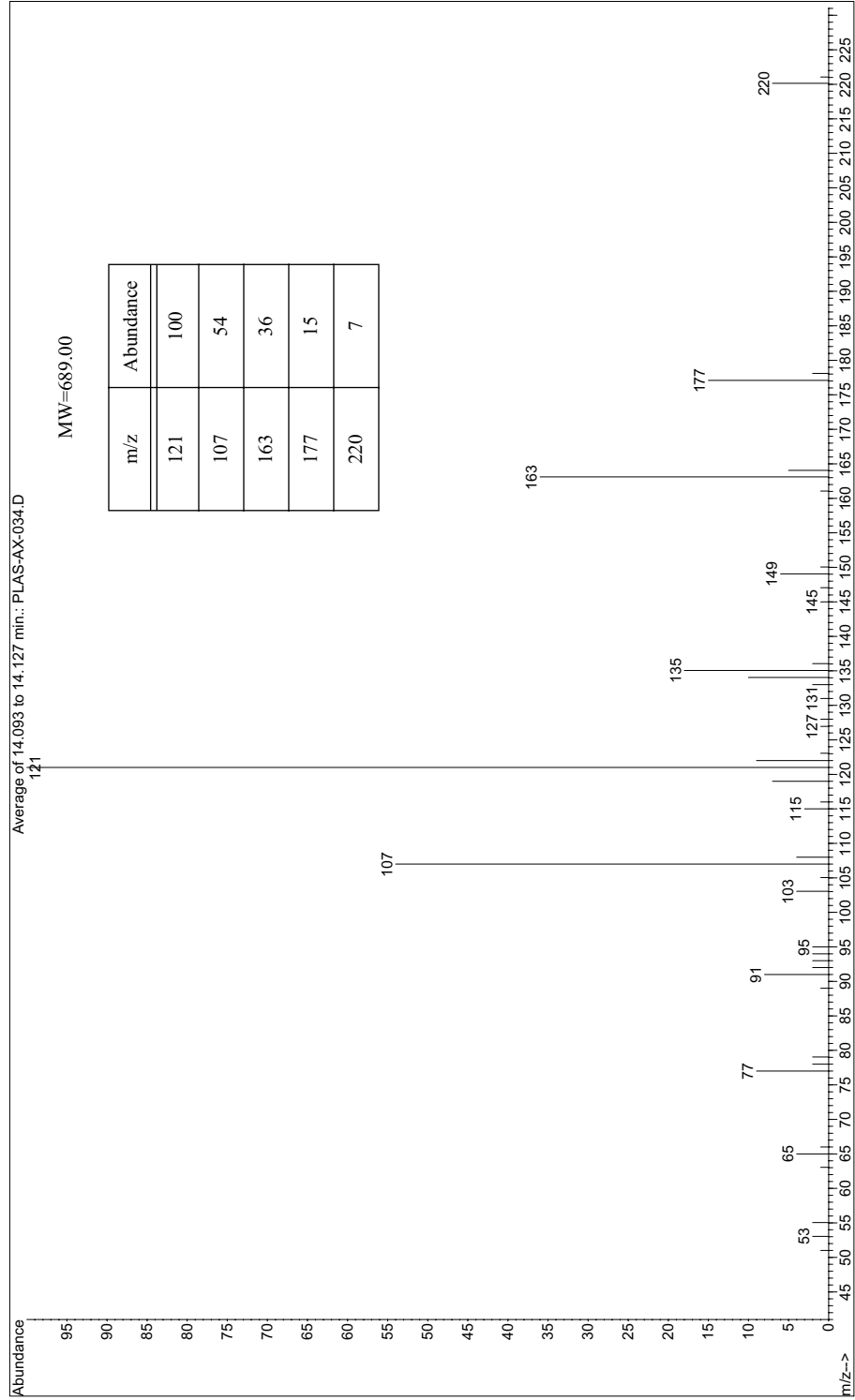
Point of Release

Can be released as point source pollution during manufacture, shipping, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

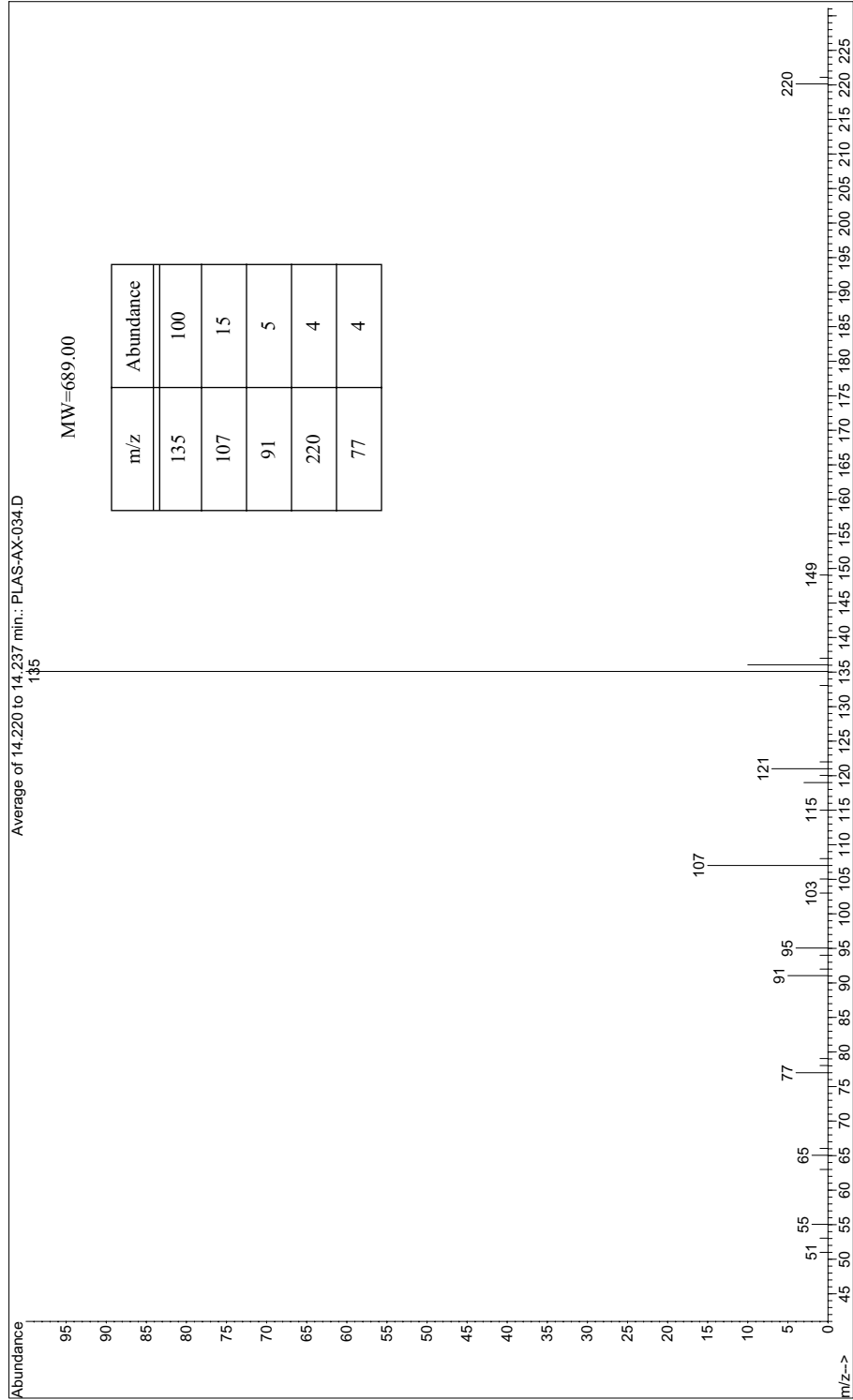
Acute toxicity: (LD50): >2000 mg/kg [Rat]. This material was not mutagenic in an Ames bacterial assay.

Mass Spectrum for Naugard® RM-51 - PLAS-AX-034



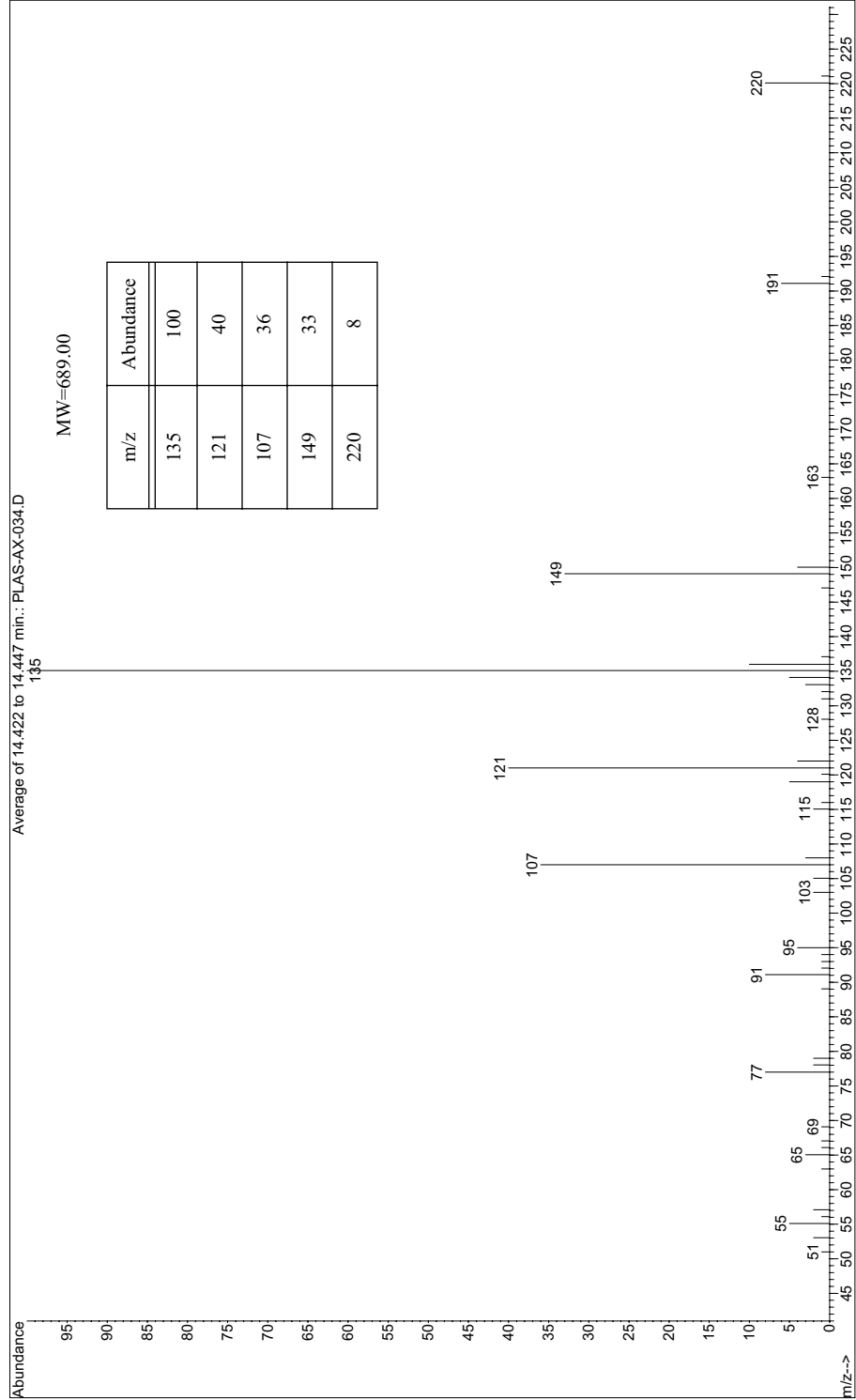
For Chromatogram See Appendix A - PLAS-AX-034 - page 515

Mass Spectrum for Naugard® RM-51 - PLAS-AX-034



For Chromatogram See Appendix A - PLAS-AX-034 - page 515

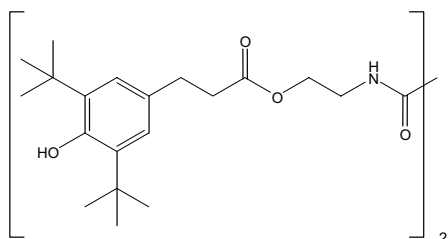
Mass Spectrum for Naugard® RM-51 - PLAS-AX-034



For Chromatogram See Appendix A - PLAS-AX-034 - page 515

Naugard® XL-1

Chemtura Corporation

**CAS Number** 70331-94-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₄₀H₆₀N₂O₈**Molecular Weight** 697**Chemical Name**

2,2'-oxamidobis[ethyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]

Synonyms

(1,2-dioxoethylene)bis(iminoethylene) bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]; 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, (1,2-dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl) ester

Brand Names & Manufacturers

Rionox MD-697

Physical Properties

Appearance	White to off-white powder or granules					
Melting Point	170-180 °C			Boiling Point	N/A	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	1.6	U	10	U	<0.1

Application, Regulatory & Environmental Information**Application**

Non-discoloring, metal deactivator and antioxidant, acts as a hindered phenolic antioxidant. Typical end use applications include wire and cable insulation, film and sheet manufacture as well as automotive parts.

Regulatory Information

FDA approved per 21CFR175.105 in food packaging adhesives and 178.2010 for use in olefin polymers in food contact at usage levels not to exceed 0.1% by weight of finished product.

Environmental Impact

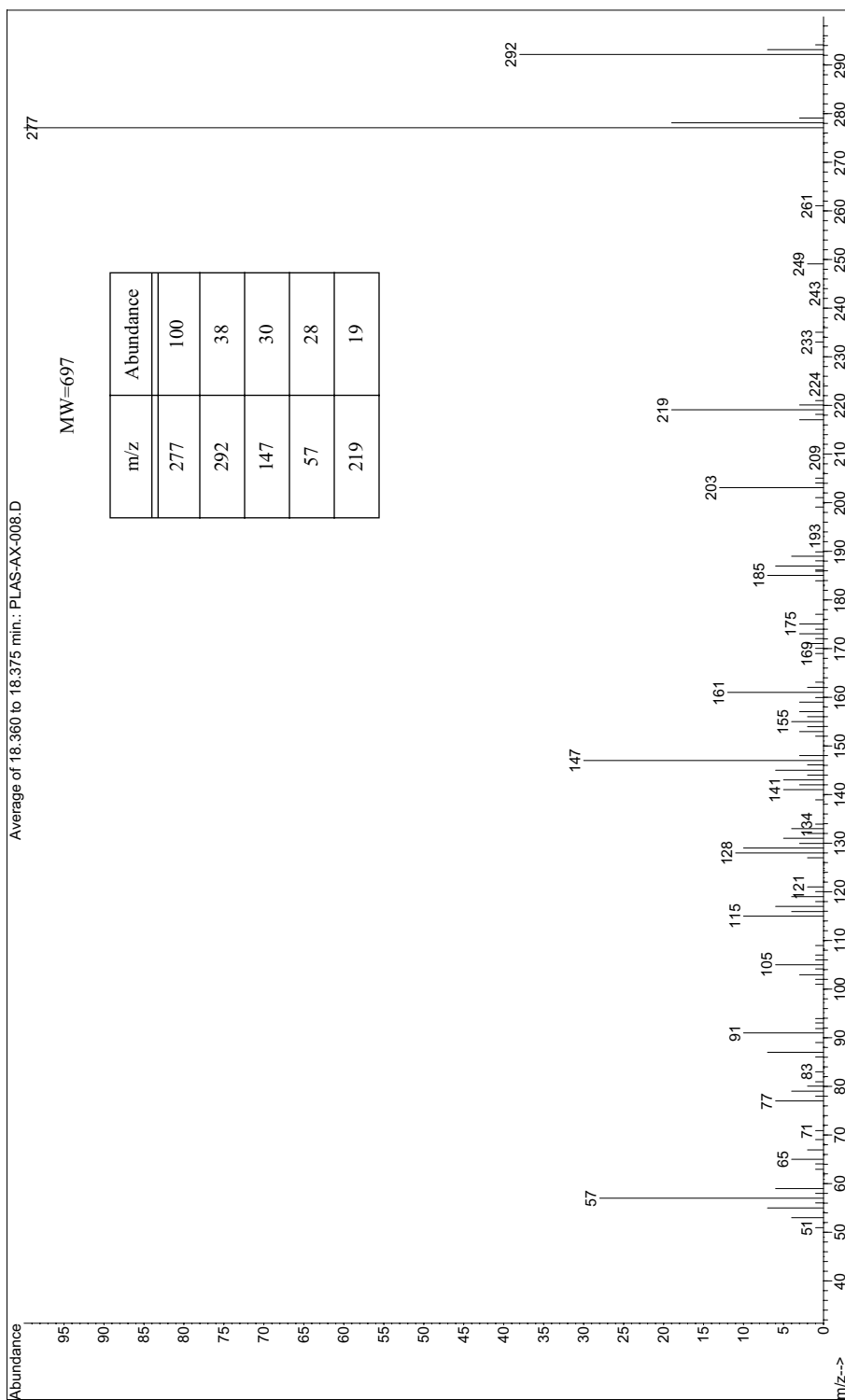
Based on test results of similar compounds, there is a high potential for this compound to bioaccumulate and be inherently toxic to aquatic wildlife.

Point of Release

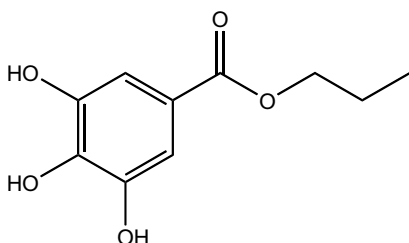
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): >10 g/kg [Rat].

Mass Spectrum for Naugard® XL-1 - PLAS-AX-008

For Chromatogram See Appendix A - PLAS-AX-008 - page 516

Propyl gallate**CAS Number** 121-79-9**RTECS Number** LW8400000**Abbreviation** Not Identified**Formula** C₁₀H₁₂O₅**Molecular Weight** 212.20**Chemical Name**

propyl 3,4,5-trihydroxybenzoate

Synonyms

3,4,5-trihydroxybenzene-1-propyl carboxylate

Brand Names & Manufacturers

Sold as bulk chemical

Varied

Physical Properties**Appearance** White to beige powder**Melting Point** 148-150 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	350	S	S	U	U	U

Application, Regulatory & Environmental Information**Application**

An antioxidant that exhibits antimicrobial activity used in olefinic thermoplastics and adhesive blends. Mainly used as antioxidant additive in fats, oleaginous foods, and medicinal preparations.

Regulatory Information

FDA 21CFR Direct and Indirect Food Contact (§166, §175, §176, §177, §184, §186)

Environmental Impact

Persistence in water and soil is low. Potential for bioaccumulation is also low.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

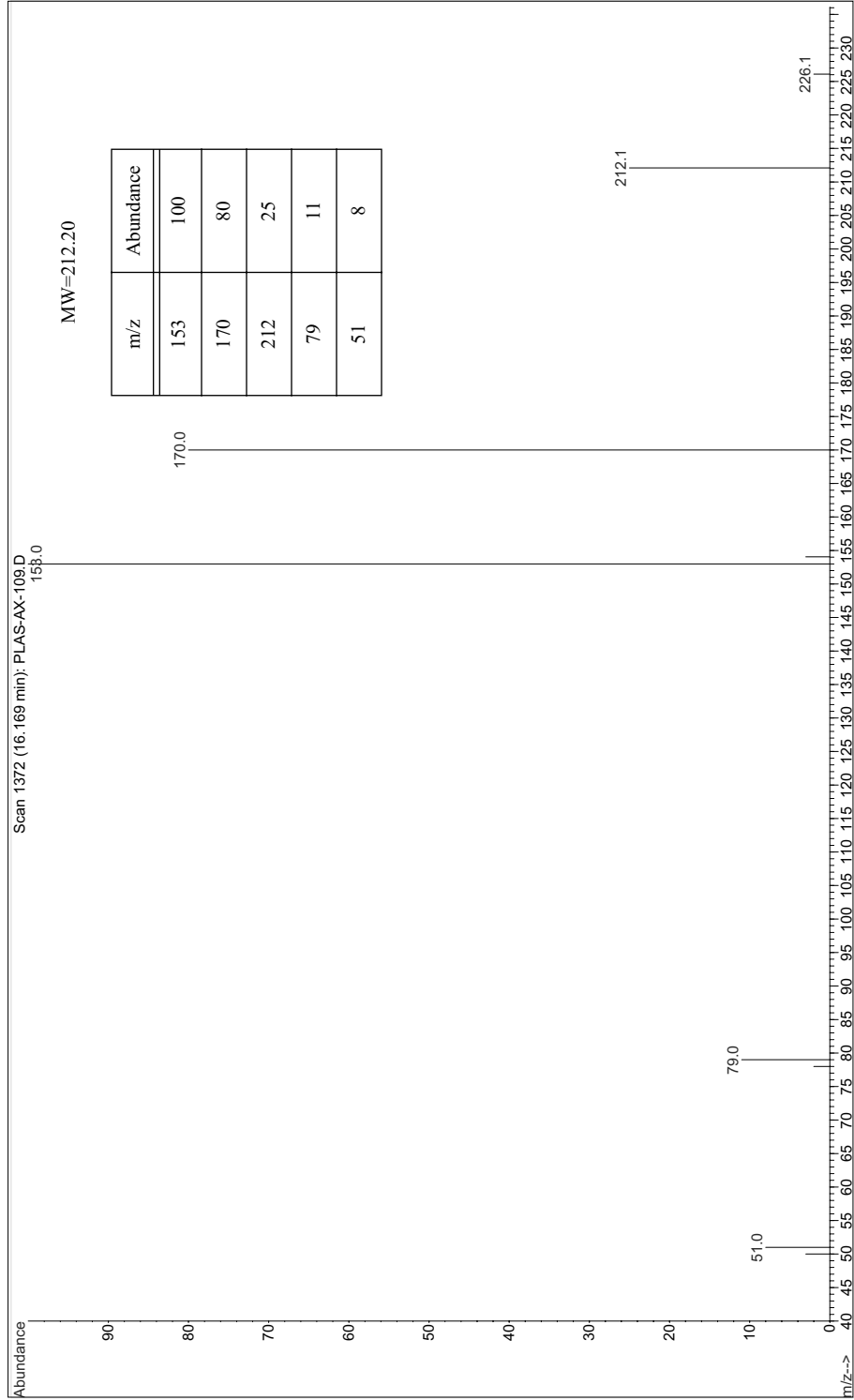
Toxicological Data

Oral (LD50): 2100 mg/kg [Rat]

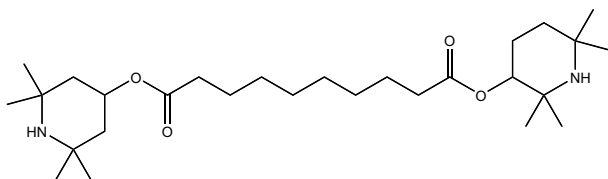
Oral (LD50): 1700 mg/kg [Mouse]

Oral (LD50): 2750 mg/kg [Rabbit]

Mass Spectrum for Propyl gallate - PLAS-AX-109



For Chromatogram See Appendix A - PLAS-AX-109 - page 517

Bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate**CAS Number** 52829-07-9**RTECS Number** HD8315000**Abbreviation** Not Identified**Formula** C₂₈H₅₂N₂O₄**Molecular Weight** 480.72**Chemical Name**

bis(2,2,6,6-tetramethylpiperidin-4-yl) decanedioate

Synonyms

decanedioic acid,1,10-bis(2,2,6,6-tetramethyl-4-piperidinyl) ester

Brand Names & Manufacturers

Adeka® LA 77

BLS® 1770

Tinuvin® 770

Adeka

Mayzo

Ciba (BASF)

Physical Properties**Appearance** Granules**Melting Point** 80-86 °C**Boiling Point** Decomposes >104 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	38	50	19	56	5

Application, Regulatory & Environmental Information**Application**

Prevents ultraviolet degradation in polypropylene, polystyrene, ABS, polyurethanes, polyacetals, and polyamides. It provides outstanding long-term stability by a radical trapping mechanism similar to that of hindered phenols. Very effective for articles with a high surface area such as films and tapes.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

LC50 (96 hour): >100 mg/L [Brachydanio Rerio]

EC50 (48 hour): 168.7 mg/L [Daphnia Magna]

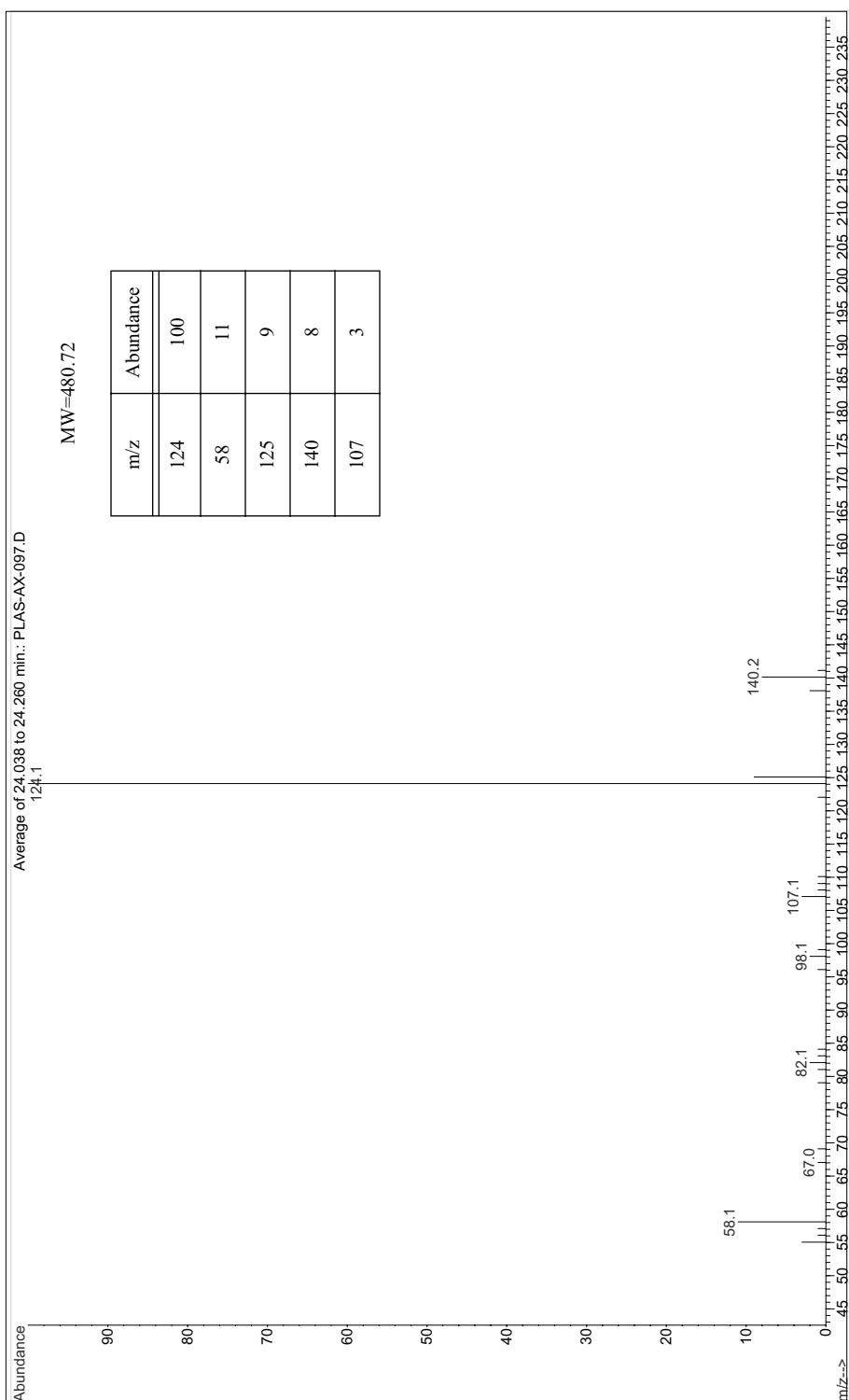
EC50: 1.9 mg/L [Algae]

Point of Release

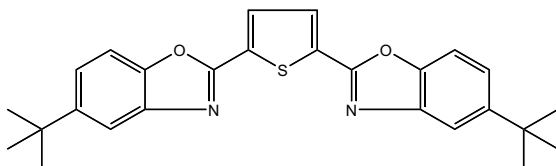
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological DataLD50 Inhalation: 500 mg/m³ (4 hour) [Rat]

Considered to be toxic if inhaled or swallowed.

Mass Spectrum for Bis(2,6,6-tetramethyl-4-piperid) sebacate - PLAS-AX-097

For Chromatogram See Appendix A - PLAS-AX-097 - page 519

2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole)**CAS Number** 7128-64-5**RTECS Number** DM4888332**Abbreviation** BBOT**Formula** C₂₆H₂₆N₂O₂S**Molecular Weight** 430.56**Chemical Name**

5-tert-butyl-2-[5-(5-tert-butyl-1,3-benzoxazol-2-yl)thiophen-2-yl]-1,3-benzoxazole

Synonyms

2,2'-(2,5-thiophenediyl)bis(5-tertiarybutylbenzoxazol)

Brand Names & Manufacturers

Benetex® OB
 Eastobrite® OB
 Sunpal OB

Mayzo, Inc.
 Eastman Chemical Company
 Sunny Chemical

Physical Properties**Appearance** Yellow to greenish powder**Melting Point** 196-202 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.05	0.06	0.2	N/A	0.2

Application, Regulatory & Environmental Information**Application**

Used as an optical brightener and to offset the yellowness of a polymer and yield a whiter appearance. Can be used in thermoplastics, coatings, printing inks, paints, dyes, manufactured fibers, synthetic leather, waxes, fats, and oils.

Regulatory Information

FDA approved for use in polymers subject to the limitations in 21 CFR §176.170(c).

Environmental Impact

Contains no hazardous air pollutants or ozone-depleting substances. It is also not listed on the US Clean Water Act Priority Pollutant List.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

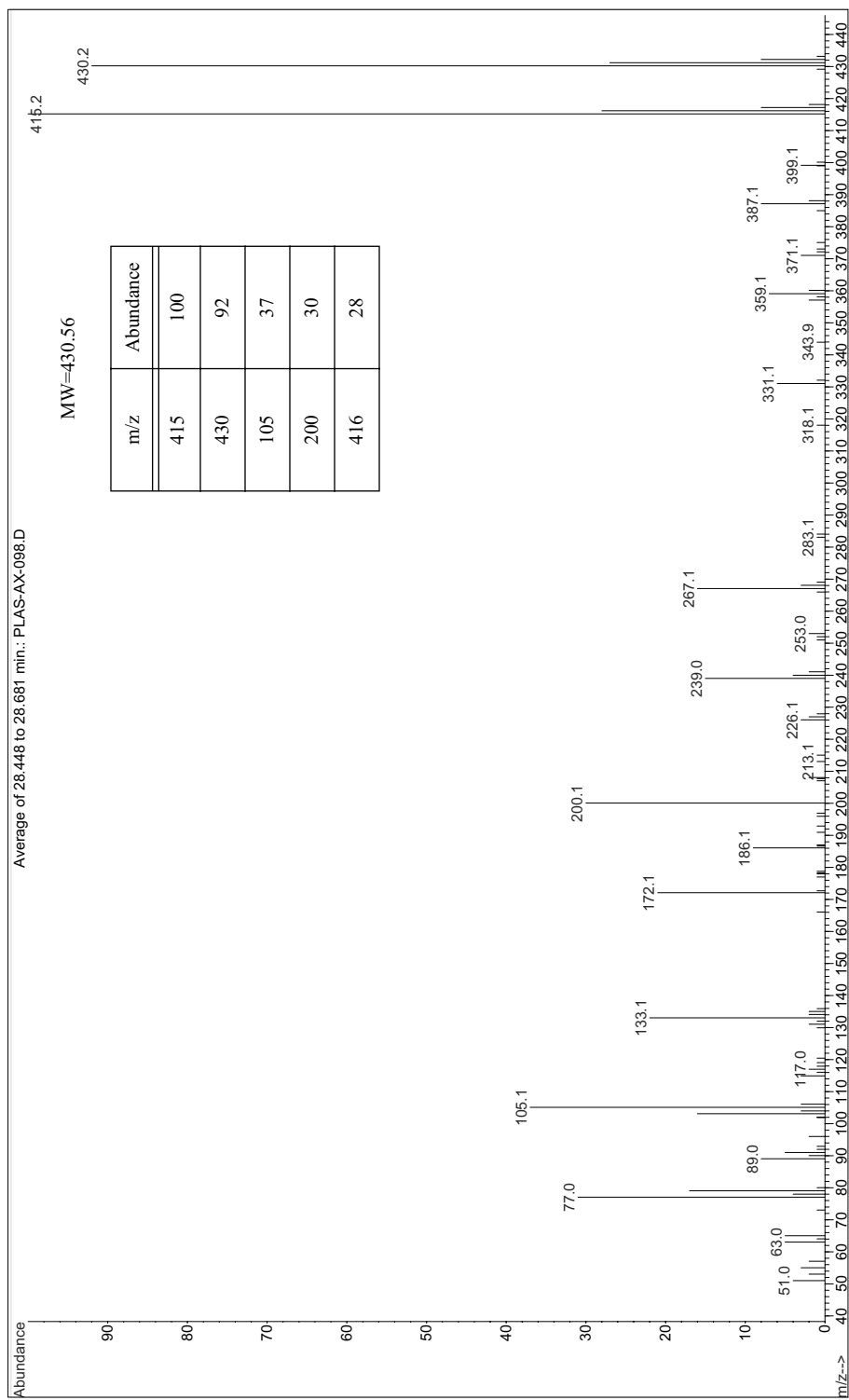
Toxicological Data

Oral (LD50): >10000 mg/kg [Rat]

Inhalation (LD50): >1.8 mg/L/4 hour [Rat]

Repeated and prolonged exposure to this product is not known to aggravate existing medical conditions.

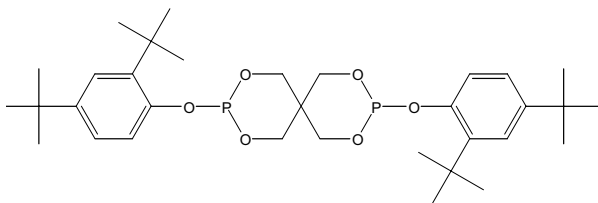
Mass Spectrum for 2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole) - PLAS-AX-098



For Chromatogram See Appendix A - PLAS-AX-098 - page 520

Ultrinox® 626

Chemtura Corporation

**CAS Number** 26741-53-7**RTECS Number** TG7400000**Abbreviation** Not Identified**Formula** C₃₃H₅₀O₆P₂**Molecular Weight** 604.69**Chemical Name**

bis(2,4-di-tert-butylphenyl)pentaerythritol diphosphite

Synonyms

bis(2,4-di-tert-butylphenyl) pentaerythritol diphosphite; 3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro(5.5) undecane

Brand Names & Manufacturers

	Chemtura Corporation	Alkanox® P24
	Albemarle	Ethaphos® 326
Irgafos® XP 60	Ciba Specialty Chemicals	

Physical Properties

Appearance	White powder or granule					
Melting Point	173-180 °C			Boiling Point	>311 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	2.1	U	11	34	7.3

Application, Regulatory & Environmental Information**Application**

Solid organophosphite antioxidant that provides color stability, reduces polymer degradation, and improves gas fading performance in many resins. It may be used in polyethylene, polypropylene, polystyrene, polyesters, elastomers, PVC, and thermoplastics.

Regulatory Information

Approved by the FDA for food contact applications under 21CFR178.2010 covering antioxidants and/or stabilizers for polymers.

Environmental Impact

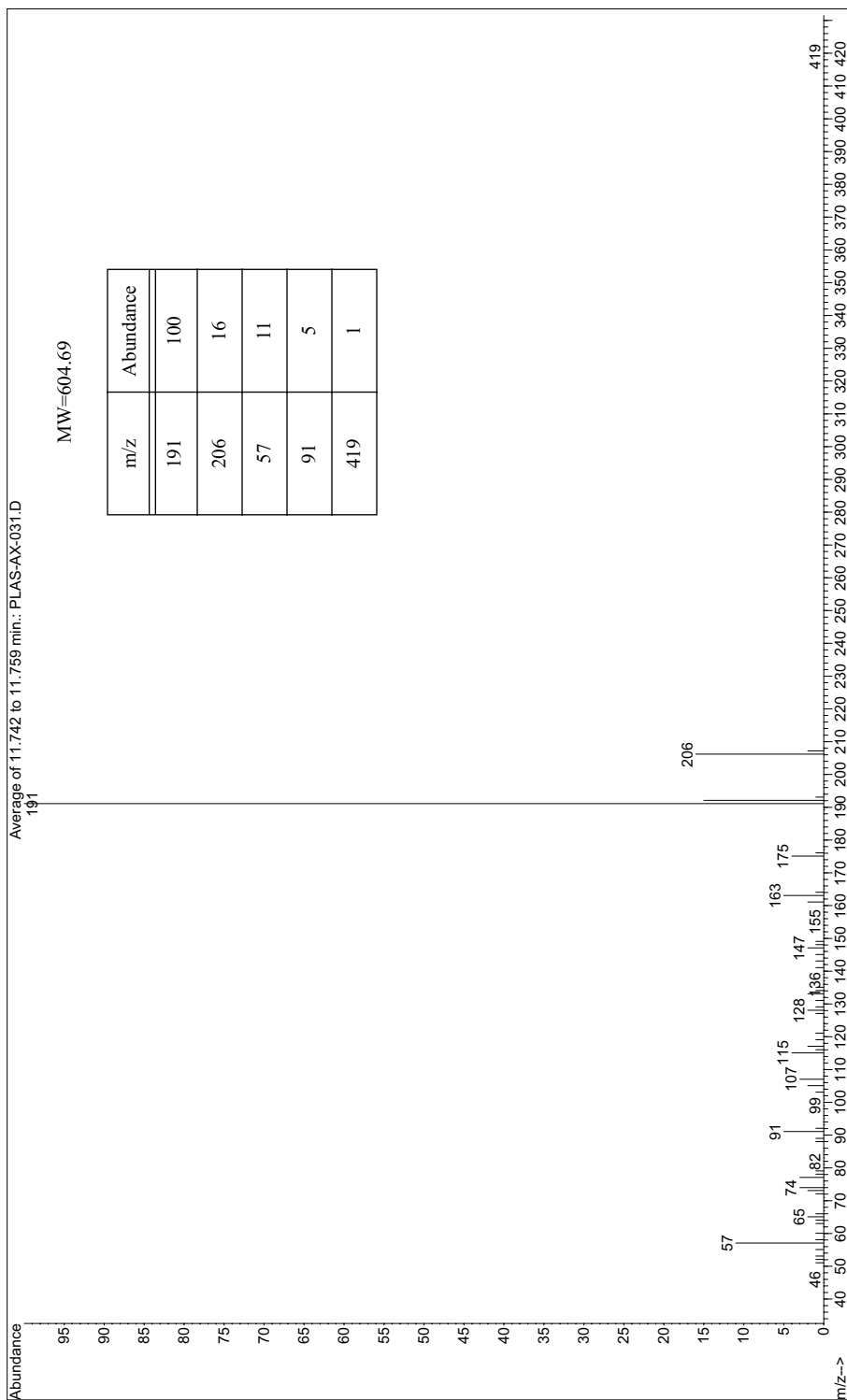
Log Pow of 10.6 indicates a high potential to bioaccumulate. This chemical is not estimated to be readily biodegradable.

Point of Release

Can be released as a point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the longevity of the products and upon disposal of the products.

Toxicological Data

Acute oral toxicity (LD50): 5580 mg/kg [Rat], acute dermal toxicity (LD50): >200 mg/kg [Rabbit].

Mass Spectrum for Ultrinox[®] 626 - PLAS-AX-031

For Chromatogram See Appendix A - PLAS-AX-031 - page 521

Coupling Agents

Coupling agents are active compounds that are capable of bonding organic polymer systems to inorganic substrates such as glass, mineral fillers, metals, and metallic oxides. In composites, the stable bond formed via the coupling agent leads to significant property-enhancing effects. Coupling agents are used in filled polymer systems, including both thermosets and thermoplastics, such as glass fiber reinforced epoxy resins, phenolics, and rubber applications.

Organosilanes [compounds of silicon and hydrogen with a molecular formula of $R_1Si(OR)_{2\text{or}3}$] are the most widely used coupling agents. The adhesion mechanism is based on two groups in the silane structure. The $Si(OR)$ portion reacts with the inorganic reinforcement, while the R_1 organofunctional (vinyl-, amino-, epoxy-, etc.) group reacts with the resin.

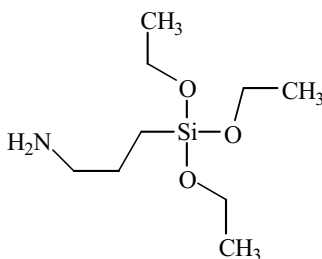
Application of coupling agents greatly improves the physical properties of the compound across a wide range of uses. Formation of a chemical bond between a polymer and an inorganic reinforcement assures stability when the compound is used in long-term wet environments. Coupling agents also stabilize a reinforced compound when exposed to repetitive mechanical forces, electrical stresses, and compressive loading. Coupling agents also enhance gas and water-permeability performance of polymer compounds. A parallel benefit of these compounds is that they aid dispersion of inorganic and metallic additives, while also reducing mixing time and energy.

Most typically, the coupling agent treatment is first applied to the inorganic component, then the treated material is blended with the host polymer. This assures the most efficient application of the coupling agent on the surface of the inorganic material.

Analysis of plastics for the presence of coupling agents is complicated by the fact that they react with the polymer and reinforcement to form a stable bond. Extraction and analysis methodology must be carefully considered.

Silquest® A-1100

General Electric Company

**CAS Number** 919-30-2**RTECS Number** TX2100000**Abbreviation** APTES**Formula** C₉H₂₃NO₃Si**Molecular Weight** 221.37**Chemical Name**

gamma-aminopropyltriethoxysilane

Synonyms

3-(triethoxysilyl)-1-propanamine; 3-(triethoxysilyl)propylamine; triethoxy(3-aminopropyl)silane

Brand Names & Manufacturers

Silquest® A-1102

General Electric Company

Physical Properties**Appearance** Clear liquid**Melting Point** <-70 °C**Boiling Point** 220 °C**Stability** Reacts rapidly with water/moisture

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application This material is used in numerous applications including various applications as coupling agents and adhesion promoters in fiberglass, adhesives and sealants, foundry resins, and in pre-treatment for coatings.

Regulatory Information

This material is not FDA approved for food contact applications.

Environmental Impact

This product is biodegradable. The reactive nature of this material destroys the parent material in any moisture-containing environment, thus limiting environmental exposure to the silane. The parent material is hydrolyzed in a spill situation; the rapid hydrolysis means that the parent silane is unlikely to be found in the environment. Bioaccumulation is not anticipated.

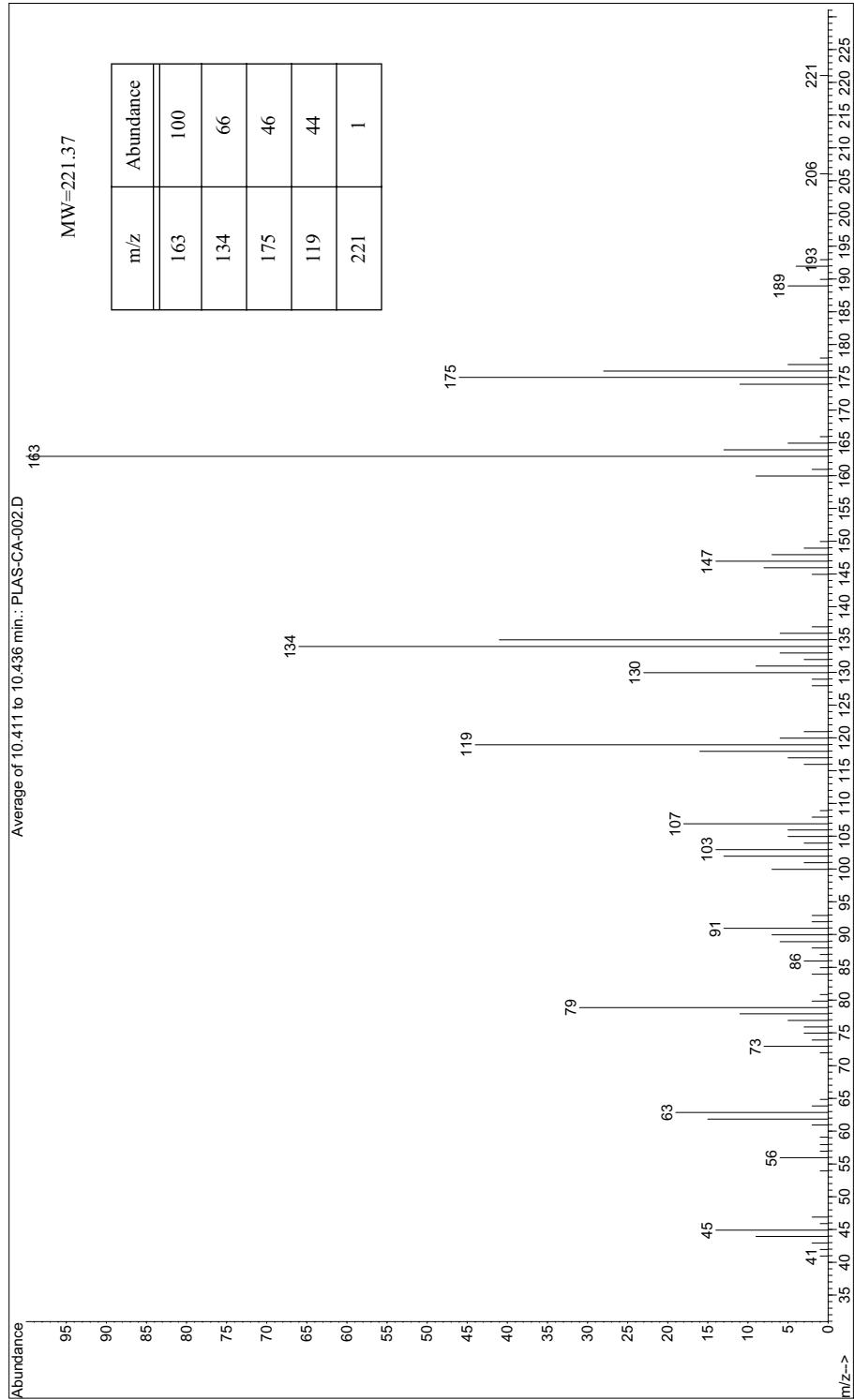
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Once APTES is added to a consumer or industrial product, the parent silane reacts with the components of the formulation and is generally present as the parent silane at 0.1–0.2% until after curing (use). After curing, the parent silane is consumed into the polymer matrix and no longer exists and greatly reduces potential for consumer or worker exposure. APTES polymerizes during use.

Toxicological Data

RTECS CLASS OF COMPOUND: Primary Irritant — toxic by ingestion. Acute oral toxicity (LD50): 1780 mg/kg [Rat]; acute dermal toxicity (LD50): 4 mL/kg [Rabbit]. Since APTES is sensitive to hydrolysis, which may occur during testing, observed toxicity is likely due to the hydrolysis products ethanol and trisilanols.

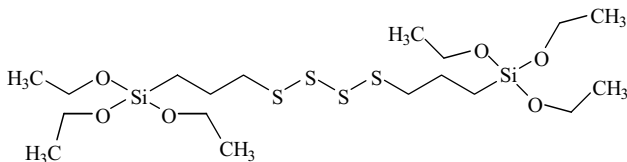
Mass Spectrum for Silquest® A-1100 - PLAS-CA-002



For Chromatogram See Appendix A - PLAS-CA-002 - page 522

Silquest® A-1289

General Electric Company

**CAS Number** 40372-72-3**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₁₈H₄₂O₆S₄Si₂**Molecular Weight** 538.94**Chemical Name**

bis-(triethoxysilylpropyl)tetrasulfide

Synonyms

N/A

Brand Names & Manufacturers

Silquest A-1289

General Electric Company

Physical Properties**Appearance** Clear light yellow liquid**Melting Point** <-78 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application Used for sulfur-cured, mineral-filled rubber applications. Silica-filled tires with lower rolling resistance, longer lasting, heat-resistant belts or hoses, and lightweight shoe soles are some of the typical uses.

Regulatory Information

This material is not FDA approved for food contact applications.

Environmental Impact

Not readily biodegradable. Acute toxicity fish: (LC50): >100 mg/L. Acute toxicity to plants: > 100 mg/L. Acute toxicity to aquatic invertebrates: (EC50): >100 mg/L.

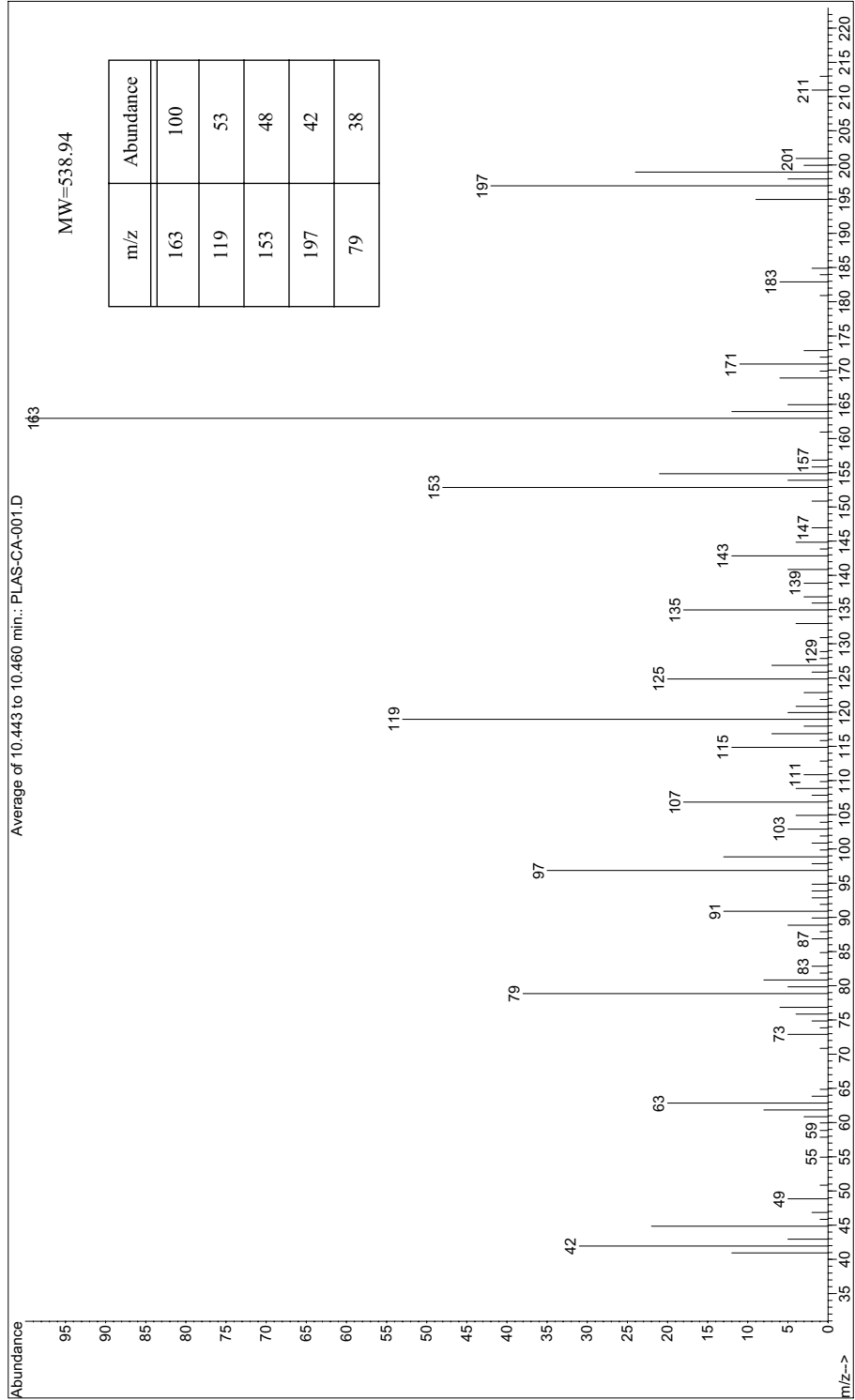
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

This product hydrolyzes in the stomach to form ethanol. Acute toxicity: Oral (LD50): >5000 mg/kg [Rat]; skin (LD50)>2000 mg/kg [Rat].

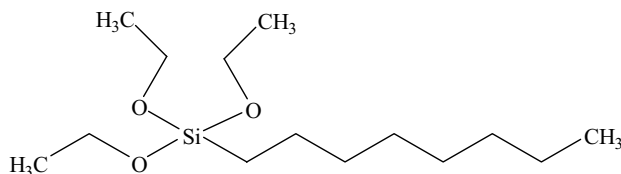
Mass Spectrum for Silquest® A-1289 - PLAS-CA-001



For Chromatogram See Appendix A - PLAS-CA-001 - page 523

Silquest® A-137

General Electric Company

**CAS Number** 2943-75-1**RTECS Number** VV6695500**Abbreviation** Not Identified**Formula** C₁₄H₃₂O₃Si**Molecular Weight** 276.55**Chemical Name**

octyltriethoxysilane

Synonyms

triethoxyoctylsilane

Brand Names & Manufacturers

Silquest A-137

General Electric Company

Physical Properties**Appearance** Clear, pale liquid**Melting Point** <-74 °C**Boiling Point** 250 °C**Stability** Reacts slowly with water.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	1-10	1-10	40-80	40-80	U

Application, Regulatory & Environmental Information**Application**

Used as a water repellent for concrete and masonry.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

Bioaccumulation is not expected to occur. Exotoxicity is expected to be low based on the reactivity with water. If spilled in the environment, the product would react with water and hydrolyze which results in highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

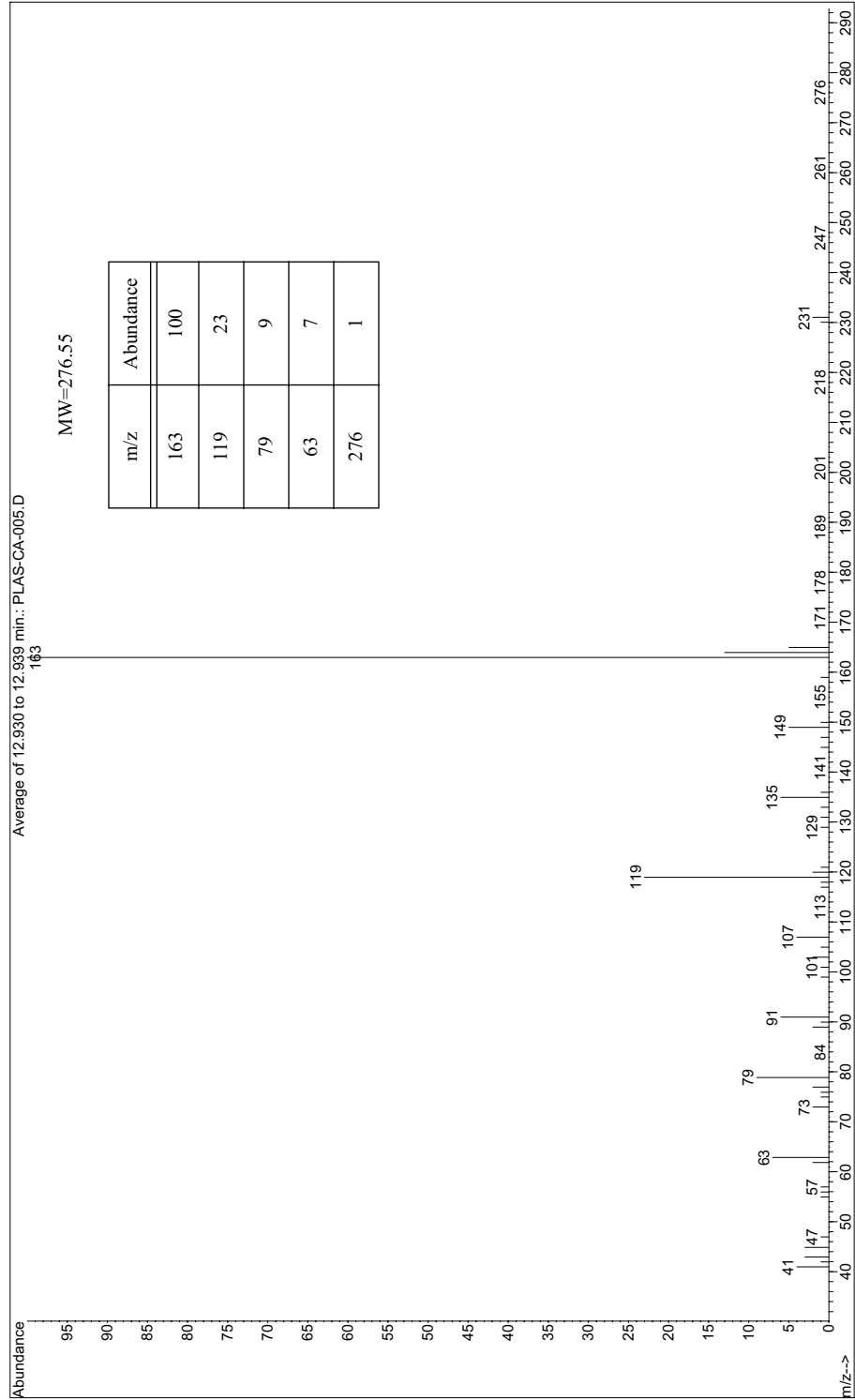
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral toxicity (LD50): >2000 mg/kg [Rat]; acute dermal toxicity (LD50): >2000 mg/kg [Rat].

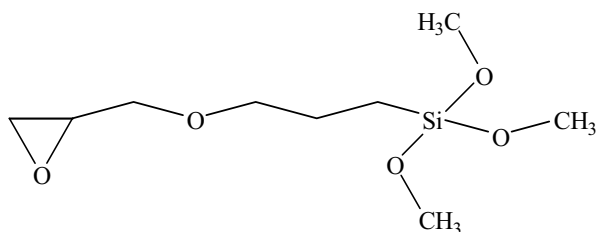
Mass Spectrum for Silquest® A-137 - PLAS-CA-005



For Chromatogram See Appendix A - PLAS-CA-005 - page 524

Silquest® A-187

Chemtura Corporation



CAS Number 2530-83-8
RTECS Number VV4025000
Abbreviation Not Identified

Formula C₉H₂₀O₅Si
Molecular Weight 236.38

Chemical Name

gamma-glycidyloxypropyltrimethoxysilane

Synonyms

3-(2,3-epoxypropoxypropyl) trimethoxysilane

Brand Names & Manufacturers

Silquest A-187

Chemtura Corporation

Physical Properties**Appearance** Clear pale liquid**Melting Point** <-70 °C**Boiling Point** 290 °C**Stability** Reacts with water/moisture.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information**Application** Used as adhesion promoter in polysulfide, urethane, epoxy, and acrylic caulks, coatings, sealants, and adhesives.**Regulatory Information**

Not approved by the FDA for applications involving implantation within the body; direct or indirect contact with the blood pathway; contact with bone, tissue, tissue fluid, or blood; or prolonged contact with mucous membranes.

Environmental Impact

Bioaccumulation is not expected to occur. Exotoxicity is expected to be low based on the reactivity with water. If spilled in the environment, the product would react with water and hydrolyze which results in highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

Point of Release

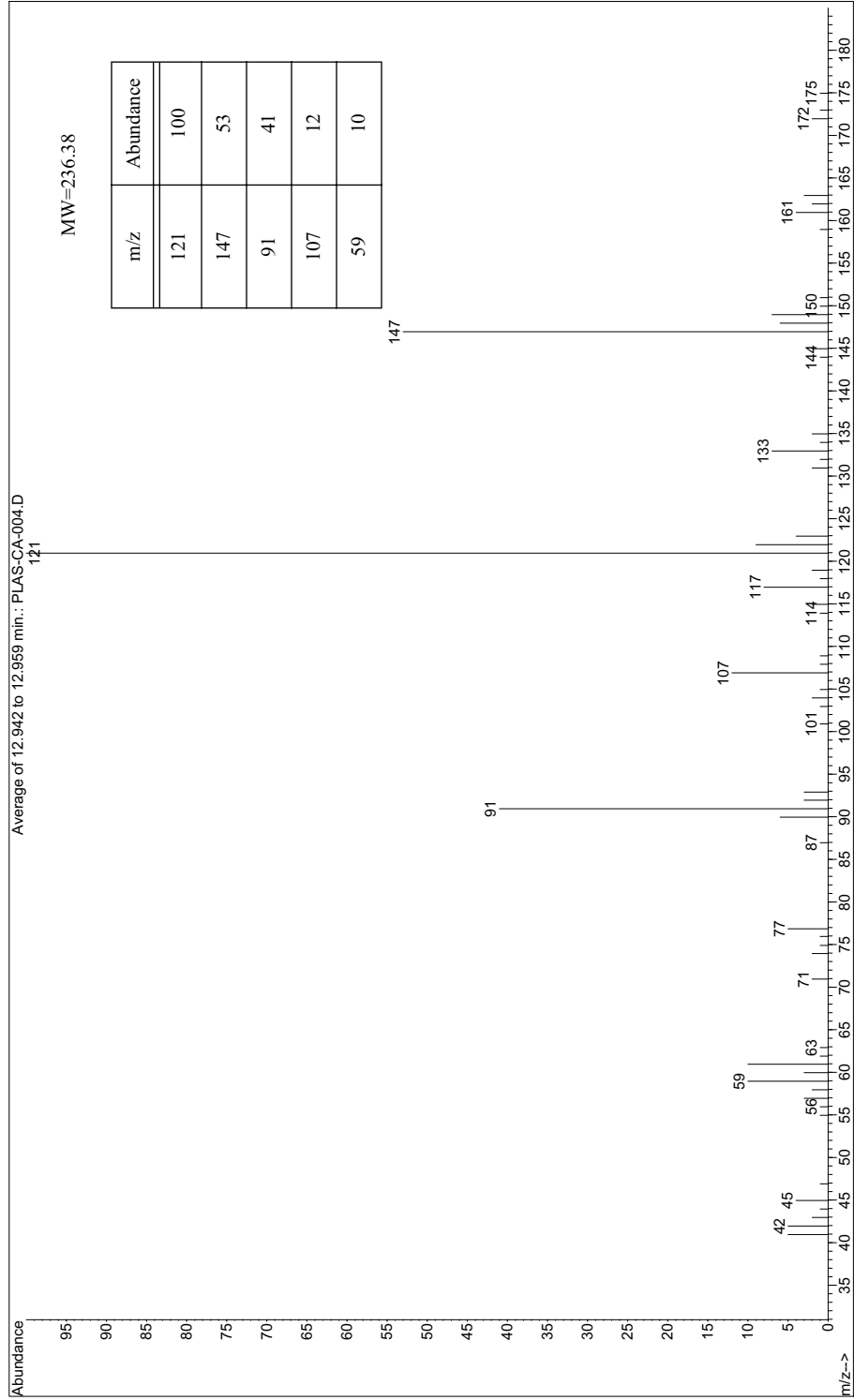
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Organometallic; mutagen; reproductive effector; primary irritant.

Acute oral toxicity (LD50): 22600 µL/kg [Rat]; acute dermal toxicity (LD50): 3970 µl/kg [Rabbit].

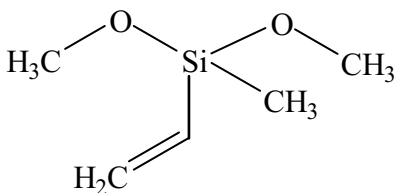
Mass Spectrum for Silquest® A-187 - PLAS-CA-004



For Chromatogram See Appendix A - PLAS-CA-004 - page 525

Silquest® A-2171

General Electric Company

**CAS Number** 16753-62-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₅H₁₂O₂Si**Molecular Weight** 132.24**Chemical Name**

vinylmethyldimethoxysilane

Synonyms

dimethoxy methylvinyl silane

Brand Names & Manufacturers

Silquest A-2171

General Electric Company

Physical Properties**Appearance** Clear pale yellow liquid**Melting Point** <0 °C**Boiling Point** 106 °C**Stability** Stable; reacts slowly with water to form methanol.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application Silquest A-2171 offers vinyl and silane functionality making it suitable for crosslinking of organic polymers. It is also useful as a crosslinker in systems where greater elongation is required. It is also recommended for chain extension of RTV silicones or other silane or HO functional polymers. The resulting Si-O-Si crosslinked sites are resistant to exposure to moisture, chemicals, and UV. Siloxane crosslinkers tend not to generate color and are resistant to environmental factors such as acid rain.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

Bioaccumulation is not expected to occur. Exotoxicity is expected to be low based on the reactivity with water. If spilled in the environment, the product would react with water and hydrolyze which results in highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

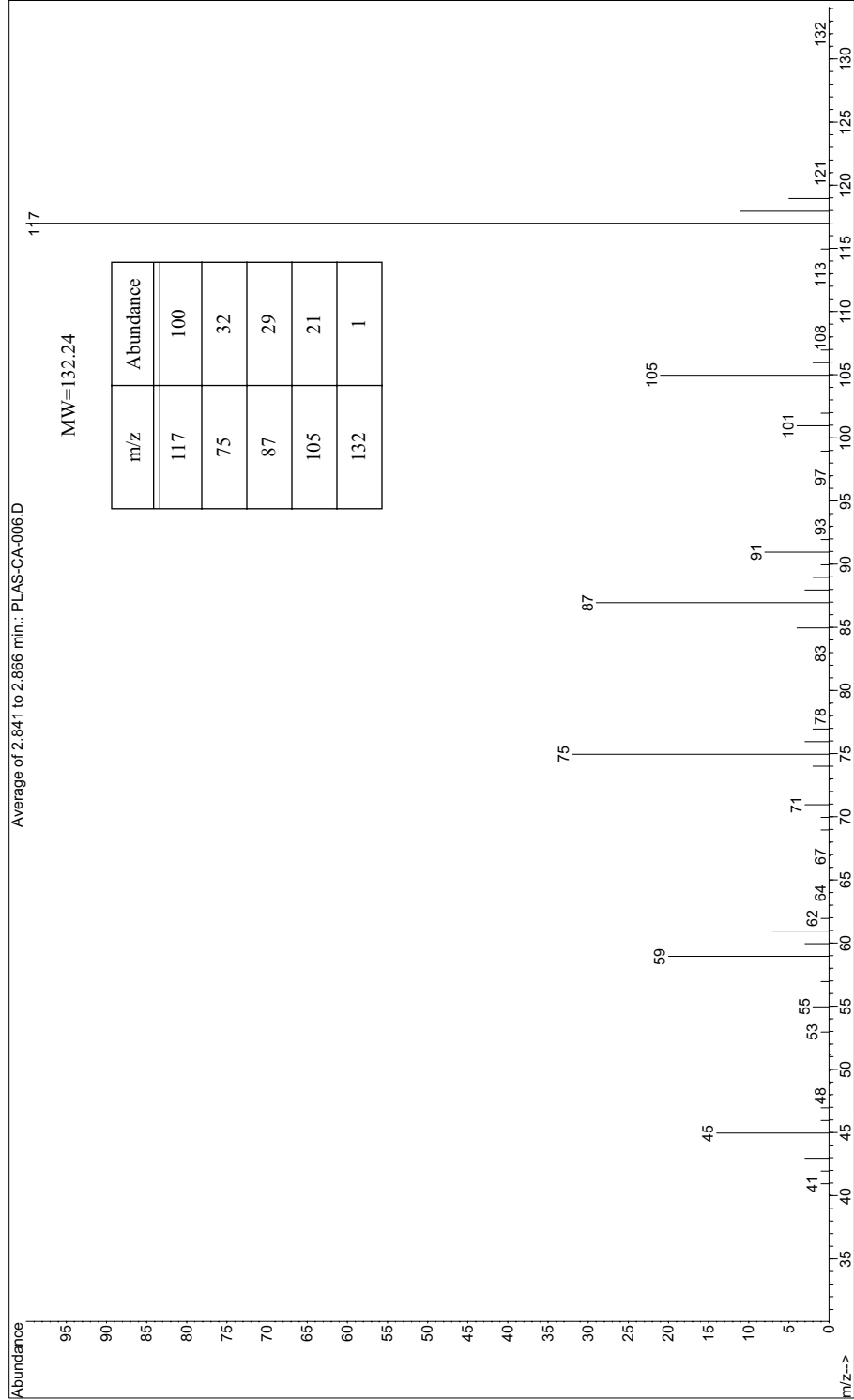
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

No adverse effects anticipated from available information. No evidence of embryotoxicity or teratogenicity. Material was not mutagenic in an Ames bacterial assay.

Mass Spectrum for Silquest® A-2171 - PLAS-CA-006



For Chromatogram See Appendix A - PLAS-CA-006 - page 526

Flame Retardants

Flame retardants are added not to aid in processing, but rather to inhibit ignition or flammability of the end-use product. They are added so that the polymer compound is able to meet flammability standards established by either mandatory government regulations or voluntary specifications.

Common flame retardants are alumina trihydrate, brominated compounds, phosphorous compounds, antimony oxide, chlorinated compounds, and boron compounds. Brominated flame retardants are preferred for thermoplastic resins such as polystyrene, polyesters, polyolefins, and polyamides but are also used in epoxies, ABS, and polycarbonates. Decabromodiphenyl oxide is one of the most common brominated flame retardants in use.

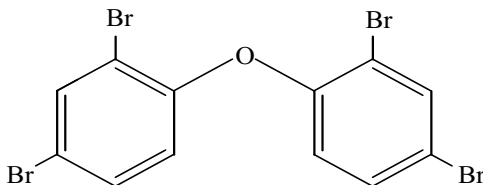
No matter the source, flame retardants, especially the polybrominated diphenyl ethers (PBDEs), are coming under scrutiny because they are persistent organic pollutants (POPs). They are appearing in human samples, most notably serum, adipose fat tissue, and breast milk. PBDEs are also under investigation as potential endocrine mimickers or endocrine disruptors. As a result, PBDEs are the most highly regulated flame retardants. Their environmental fate will continue to be a topic of research for years to come.

Chlorinated hydrocarbons have also found wide use as flame retardant additives for polymers. Some of these may not be obvious as flame retardants since they were most commonly used as insecticides. Examples include chlordane and Mirex. These are also toxic and bioaccumulative and have been banned from manufacture as a result.

From an analytical view, these materials have very distinct structures and mass spectra for which a positive identification is assured. These compounds typically resist dissolution and lend themselves to thermal desorption sampling for GC/MS analysis.

2,2',4,4'-Tetrabromodiphenyl ether

AccuStandard, Inc.

**CAS Number** 40088-47-9**RTECS Number** DA6630000**Abbreviation** BDE-47**Formula** C₁₂H₆Br₄O**Molecular Weight** 485.82**Chemical Name**

2,2',4,4'-tetrabromodiphenyl ether

Synonyms

BDE-47; tetrabromodiphenyl ether; PBDE-47

Application

BDE-47 was a component of many commonly used flame retardants, including PeBDE, DE-71, Bromkal 70-5DE, and other popular mixtures. DE-71 was sold by Great Lakes Chemical Corporation as a flame retardant for unsaturated polyester, rigid and flexible polyurethane foams, epoxies, laminates, adhesives, and coatings. This material was phased out at the end of 2004. It typically contained somewhere between 20 and 50% BDE-47.

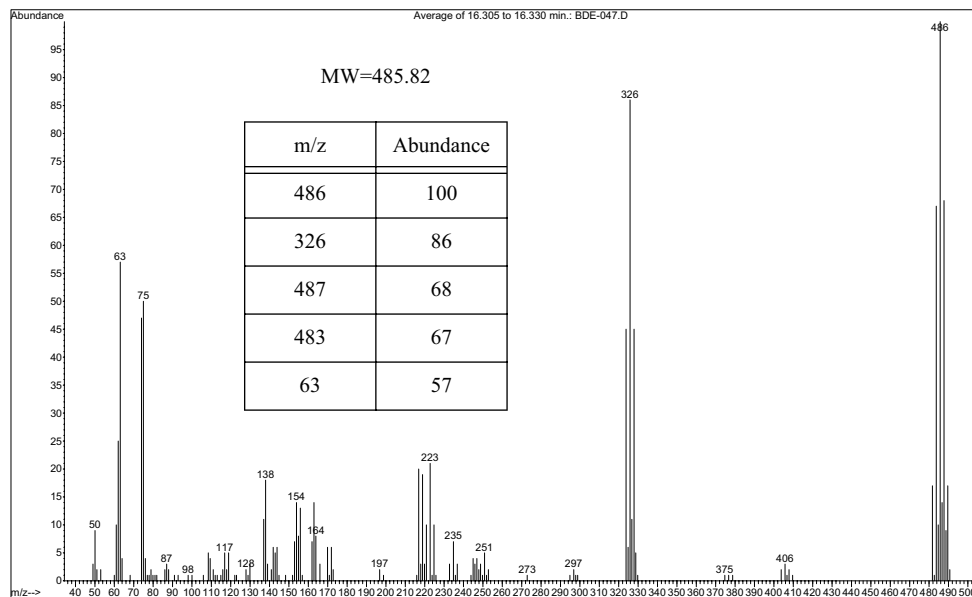
Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-047 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

Toxicological and Environmental Data

BDE-47 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research. It is biologically persistent, and has a high bioaccumulation potential. It is under investigation as an endocrine disruptor and studies for human health concerns are ongoing.

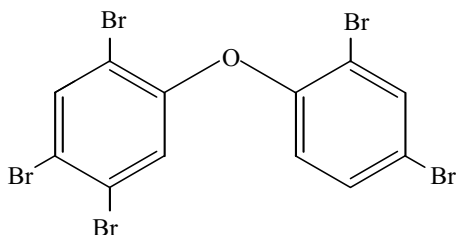
Acute oral toxicity (LD50): >500 mg/kg [Rat].



For Chromatogram See Appendix A - BDE-047 - page 527

2,2',4,4',5-Pentabromodiphenyl ether

AccuStandard, Inc.

**CAS Number** 32534-81-9**RTECS Number** DD6625350**Abbreviation** BDE-99**Formula** C₁₂H₅Br₅O**Molecular Weight** 564.72**Chemical Name**

2,2',4,4',5-pentabromodiphenyl ether

Synonyms

BDE-99; pentabromodiphenyl ether; PBDE-99

Application

BDE-99 was a component of many commonly used flame retardants, including DE-71, Bromkal G1, and other popular mixtures. DE-71 was sold by Great Lakes Chemical Corporation as a flame retardant for unsaturated polyester, rigid and flexible polyurethane foams, epoxies, laminates, adhesives, and coatings. This material was phased out at the end of 2004. It typically contained about 50% BDE-99.

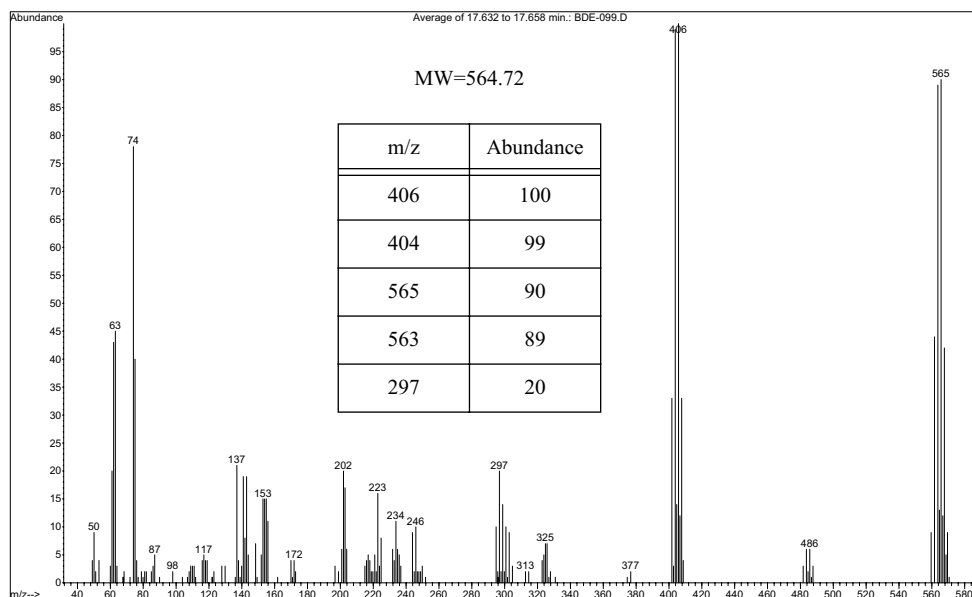
Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-099 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

Toxicological and Environmental Data

Classified as a persistent organic pollutant, which can bioaccumulate through the food web, and pose a risk of causing adverse effects to human health and the environment.

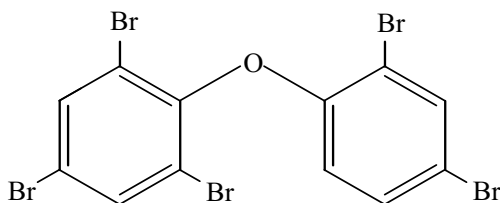
Acute oral toxicity (LD50): 5 gm/kg [Rat]; acute dermal toxicity (LD50): 2 gm/kg/24 hour [Rabbit].



For Chromatogram See Appendix A - BDE-099 - page 528

2,2',4,4',6-Pentabromodiphenyl ether

AccuStandard, Inc.

**CAS Number** 189084-64-8**RTECS Number** N/A**Abbreviation** BDE-100**Formula** C₁₂H₅Br₅O**Molecular Weight** 564.69**Chemical Name**

2,2',4,4',6-pentabromodiphenyl ether

Synonyms

BDE-100

Application

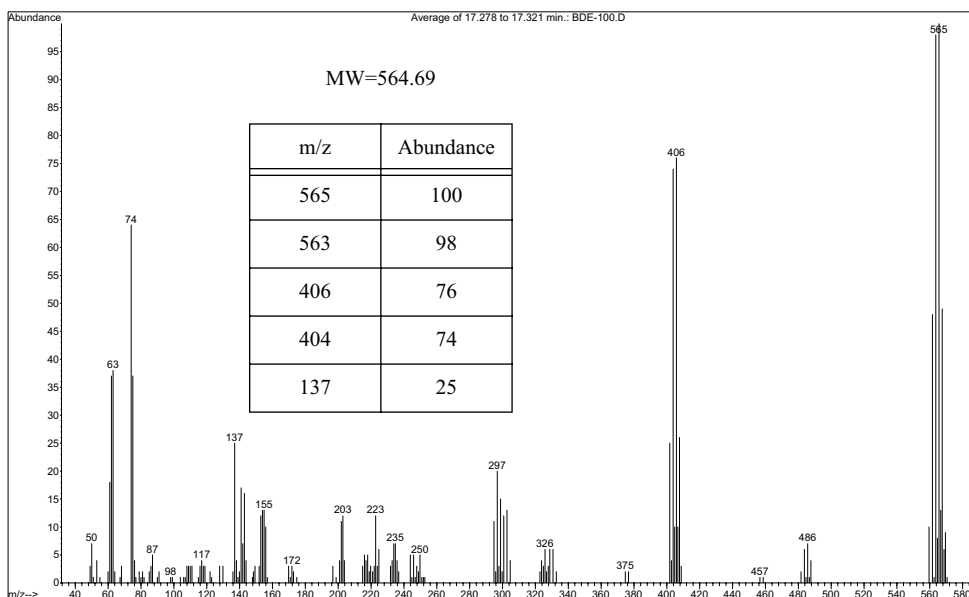
BDE-100 is a primary component of Penta-BDE which was mainly used as a flame retardant in polyurethane foam and textile applications. Penta-BDE is primarily used in North America. BDE-100 was also present in DE-71, at about 10%.

Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-100 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

Toxicological and Environmental Data

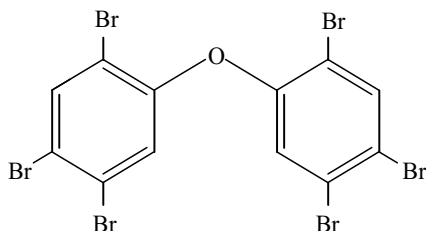
BDE-100 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research. It is biologically persistent, and has a high bioaccumulation potential. It is under investigation as an endocrine disruptor and studies for human health concerns are ongoing.



For Chromatogram See Appendix A - BDE-100 - page 529

2,2',4,4',5,5'-Hexabromodiphenyl ether

AccuStandard, Inc.

**CAS Number** 68631-49-2**RTECS Number** DA6620000**Abbreviation** BDE-153**Formula** C₁₂H₄Br₆O**Molecular Weight** 643.62**Chemical Name**

2,2',4,4',5,5'-hexabromodiphenyl ether

Synonyms

BDE-153

Application

BDE-153 occurs primarily in the commercial Octa and Penta BDE mixtures. The Octa mix contains approximately 10 to 12% hexabrominated diphenyl ethers. Penta generally contained about 4 to 8% hexabrominated diphenyl ethers including BDE-153. Typical analysis shows that the Penta mix contains an equal distribution of BDE-153 and BDE-154. The commercial Penta mix was typically used in flexible polyurethane foam for furniture and cushions. It was also used in polyesters, and epoxy and phenolic resins. Octa is used primarily in rigid plastics for housing electronics.

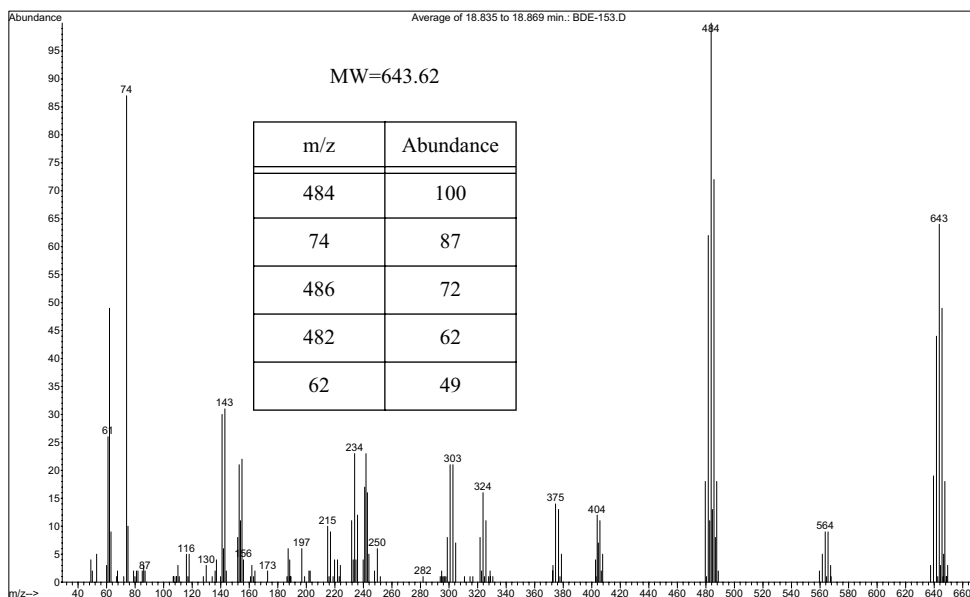
Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-153 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

Toxicological and Environmental Data

BDE-153 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research. It is biologically persistent, and has a high bioaccumulation potential. It is under investigation as an endocrine disruptor and studies for human health concerns are ongoing.

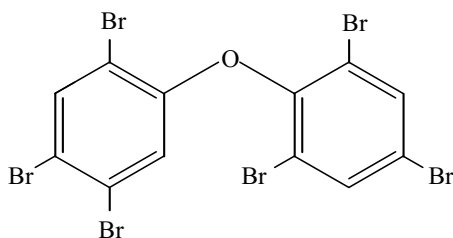
Acute oral toxicity (LD50): >500 mg/kg [Rat].



For Chromatogram See Appendix A - BDE-153 - page 530

2,2',4,4',5,6'-Hexabromodiphenyl ether

AccuStandard, Inc.

**CAS Number** 207122-15-4**RTECS Number** N/A**Abbreviation** BDE-154**Formula** C₁₂H₄Br₆O**Molecular Weight** 643.59**Chemical Name**

2,2',4,4',5,6'-Hexabromodiphenyl ether

Synonyms

BDE-154

Application

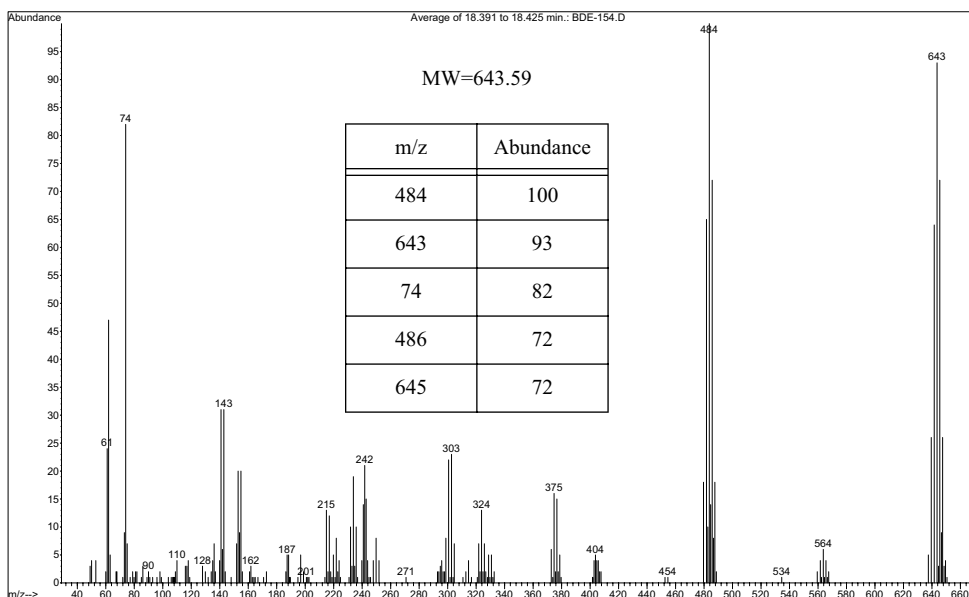
BDE-154 is a component of the commercially available octa-BDE, which is a complex mixture consisting typically of ~0.5% pentabromodiphenyl ether isomers, ~12% hexabromodiphenyl ether isomers, ~45% heptabromodiphenyl ether isomers, ~33% octaBDE isomers, ~10% nonabromodiphenyl ether isomers, and ~0.7% decabromodiphenyl ether. It is used as a flame retardant in plastics for electrical and electronic equipment.

Regulatory Information

USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS and USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS.

Toxicological and Environmental Data

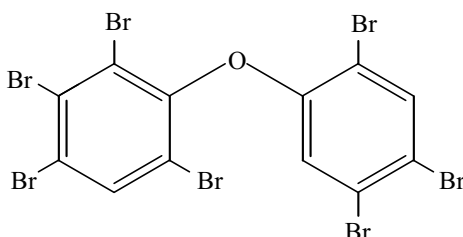
Classified as a persistent organic pollutant, which can bioaccumulate through the food web, and pose a risk of causing adverse effects to human health and the environment. BDE-154 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research.



For Chromatogram See Appendix A - BDE-154 - page 531

2,2',3,4,4',5',6-Heptabromodiphenyl ether

AccuStandard, Inc.



CAS Number 207122-16-5

RTECS Number N/A

Abbreviation BDE-183

Formula C₁₂H₃Br₇O

Molecular Weight 722.48

Chemical Name

2,2',3,4,4',5',6-heptabromodiphenyl ether

Synonyms

Synonym:
BDE-183

Application

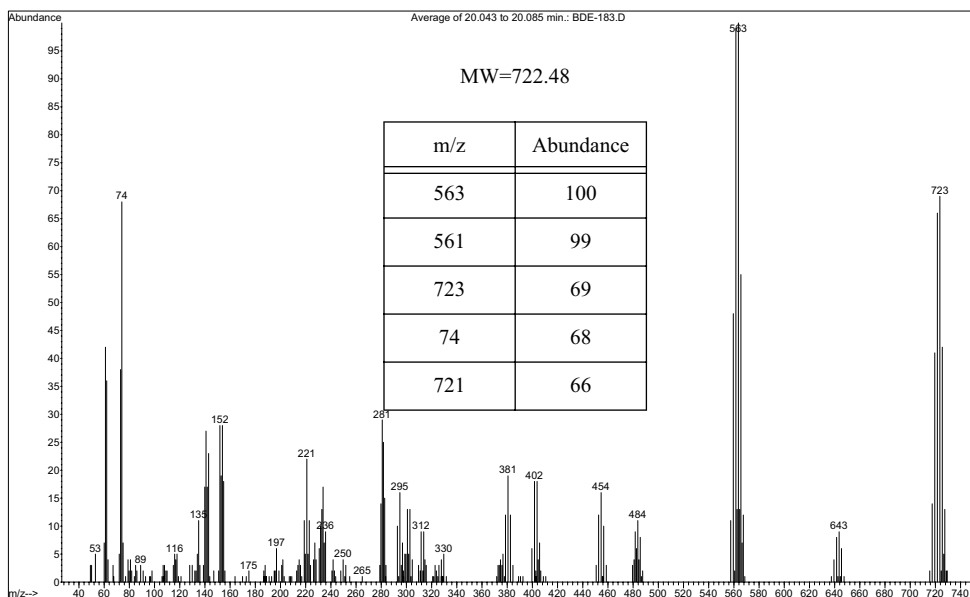
Application: BDE-183 is a major component of the commercial octa-BDE, which is a complex mixture consisting typically of ~0.5% pentabromodiphenyl ether isomers, ~12% hexabromodiphenyl ether isomers, ~45% heptabromodiphenyl ether isomers, ~33% octaBDE isomers, ~10% nonabromodiphenyl ether isomers, and ~0.7% decabromodiphenyl ether. It is used as a flame retardant in plastics for electrical and electronic equipment.

Regulatory Information

USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS, California Method 750-M and USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS.

Toxicological and Environmental Data

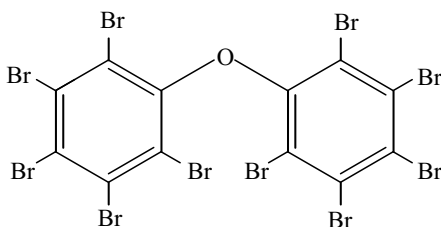
Classified as a persistent organic pollutant, which can bioaccumulate through the food web, and pose a risk of causing adverse effects to human health and the environment. BDE-154 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research.



For Chromatogram See Appendix A - BDE-183 - page 532

Decabromodiphenyl ether

AccuStandard, Inc.

**CAS Number** 1163-19-5**RTECS Number** KN3525000**Abbreviation** BDE-209**Formula** C₁₂Br₁₀O**Molecular Weight** 959.22**Chemical Name**

decabromodiphenyl ether

Synonyms

BDE-209

Application

Deca-BDE is the most common of all the commercial BDE flame retardants. The commercial Deca is generally 95% or more of the BDE-209 congener. It is primarily used as a flame retardant in the hard, dense plastics of consumer electronics products and in the latex back coating of flame retardant upholstery textiles. It can be found in many different polymers including polycarbonates, polyesters, polyolefins, ABS, polyamides, PVC, and rubbers.

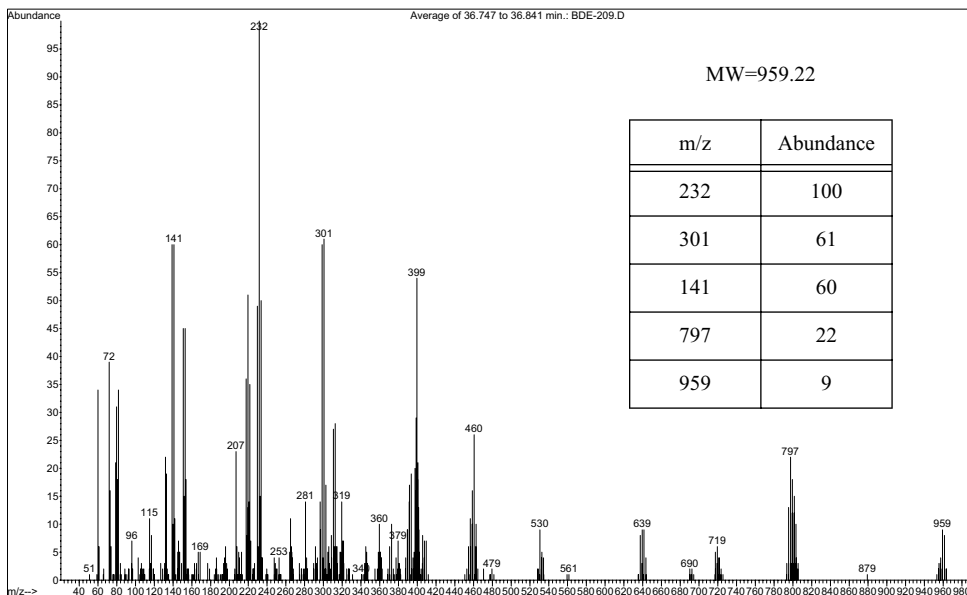
Regulatory Information

USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. BDE-209 Regulated RoHS/WEEE Regulations (2002/95/EC). Deca-BDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

Toxicological and Environmental Data

RTECS CLASS OF COMPOUND: Tumorigen; reproductive effector; primary irritant.

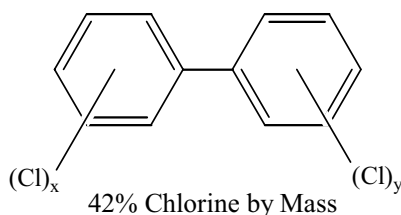
Acute oral toxicity (LD50): 2 gm/kg [Rat], acute dermal toxicity (LD50): 2 gm/kg/24 hour [Rabbit].



For Chromatogram See Appendix A - BDE-209 - page 533

Aroclor 1242

Monsanto

**CAS Number** 53469-21-9**RTECS Number** TQ1356000**Abbreviation** Not Identified**Formula** Technical mixture**Molecular Weight** N/A**Chemical Name**

N/A

Synonyms

chlorodiphenyl (42% Cl)

Application

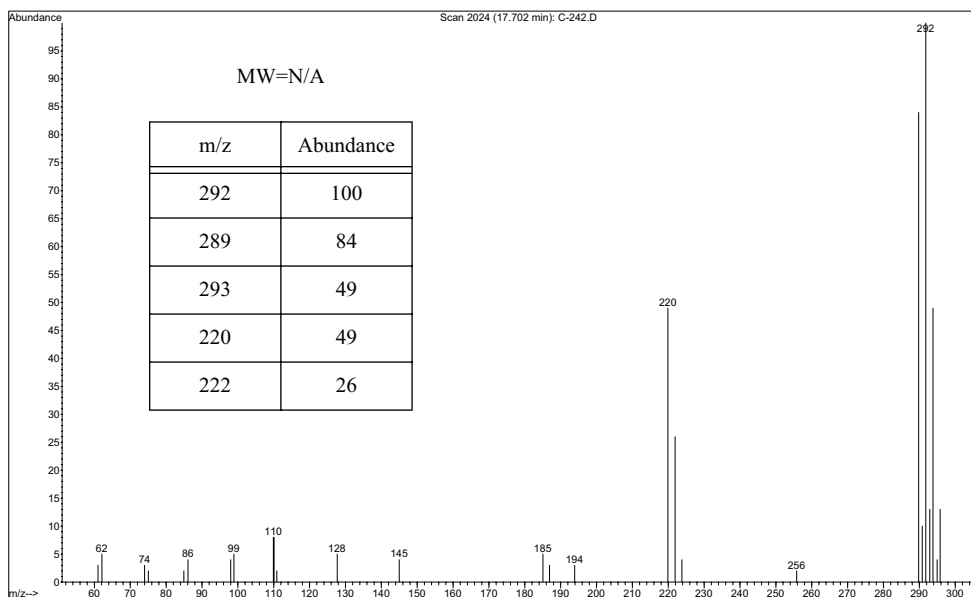
Used in electrical capacitors, electrical transformers, vacuum pumps, and gas-transmission turbines. Formerly used as heat transfer fluid, hydraulic fluids, rubber plasticizer, and in carbonless paper, adhesives, and wax extenders. Although the production and sale was discontinued in late 1977, it is still present in transformers and capacitors now in use.

Regulatory Information

Section 6(e) of the Toxic Substances Control Act (TSCA) prohibits the manufacture, processing, and distribution in commerce of PCBs. In addition, the EPA has set a limit of 0.0005 mg of PCBs per liter of drinking water (0.0005 mg/L). Discharges, spills, or accidental releases of 1 lb or more of PCBs into the environment must be reported to the EPA. The Food and Drug Administration (FDA) requires that infant foods, eggs, milk and other dairy products, fish and shellfish, poultry, and red meat contain no more than 0.2 to 3 parts of PCBs per million (0.2 to 3 ppm) of food.

Toxicological and Environmental Data

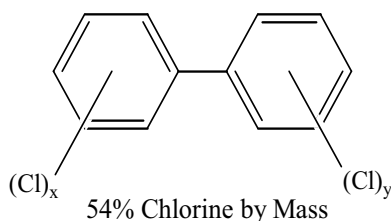
PCBs do not readily break down in the environment and thus may remain there for very long periods of time. PCBs can travel long distances in the air and be deposited in areas far away from where they were released. In water, a small amount of PCBs may remain dissolved, but most stick to organic particles and bottom sediments. PCBs also bind strongly to soil. PCBs are taken up by small organisms and fish in water and accumulate up the food chain in fish and marine mammals.



For Chromatogram See Appendix A - C-242 - page 534

Aroclor 1254

Monsanto

**CAS Number** 11097-69-1**RTECS Number** TQ1360000**Abbreviation** Not Identified**Formula** Technical mixture**Molecular Weight** Not applicable**Chemical Name**

N/A

Synonyms

chlorodiphenyl (54% Cl)

Application

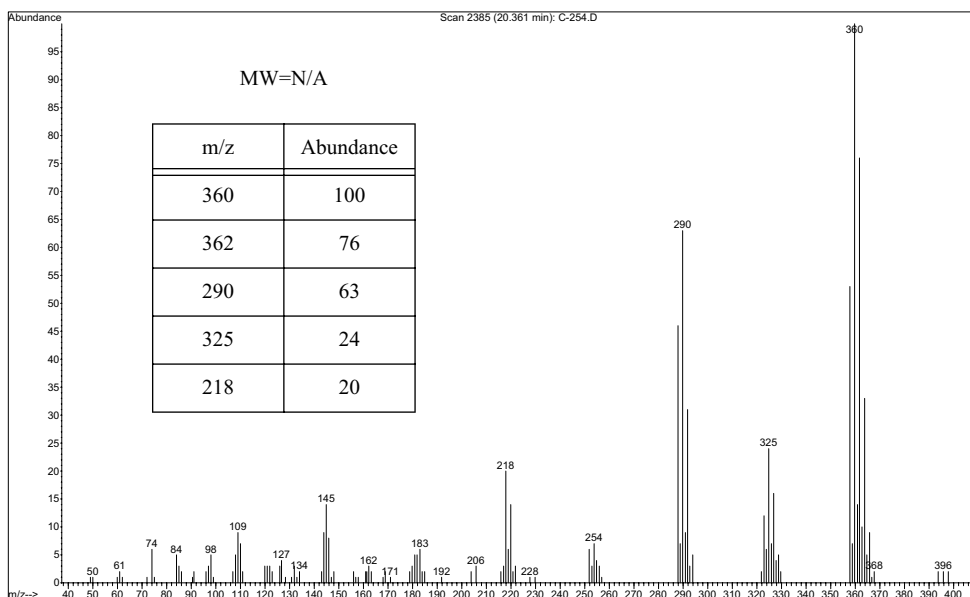
Formerly used in hydraulic fluid, rubber plasticizers, synthetic resin plasticizers, adhesives, wax extenders, dedusting agents, inks, cutting oils, pesticide extenders, sealants, and caulking compounds. Although the production and sales were discontinued in late 1977, it is still present in transformers now in use, as well as in electrical capacitors, electrical transformers, vacuum pumps, and gas-transmission turbines.

Regulatory Information

Section 6(e) of the Toxic Substances Control Act (TSCA) prohibits the manufacture, processing, and distribution in commerce of PCBs. In addition, the EPA has set a limit of 0.0005 mg of PCBs per liter of drinking water (0.0005 mg/L). Discharges, spills, or accidental releases of 1 lb or more of PCBs into the environment must be reported to the EPA. The Food and Drug Administration (FDA) requires that infant foods, eggs, milk and other dairy products, fish and shellfish, poultry, and red meat contain no more than 0.2 to 3 parts of PCBs per million parts (0.2 to 3 ppm) of food.

Toxicological and Environmental Data

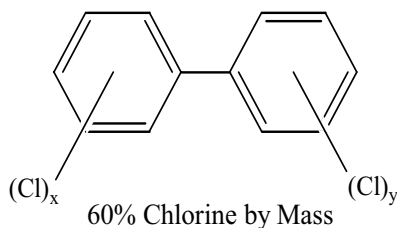
PCBs do not readily break down in the environment and thus may remain there for very long periods of time. PCBs can travel long distances in the air and be deposited in areas far away from where they were released. In water, a small amount of PCBs may remain dissolved, but most stick to organic particles and bottom sediments. PCBs also bind strongly to soil. PCBs are taken up by small organisms and fish in water and accumulate up the food chain in fish and marine mammals.



For Chromatogram See Appendix A - C-254 - page 535

Aroclor 1260

Monsanto

**CAS Number** 53469-21-9**RTECS Number** TQ1362000**Abbreviation** Not Identified**Formula** Technical mixture**Molecular Weight** Not applicable**Chemical Name**

Not applicable

Synonyms

chlorodiphenyl (42% Cl)

Application

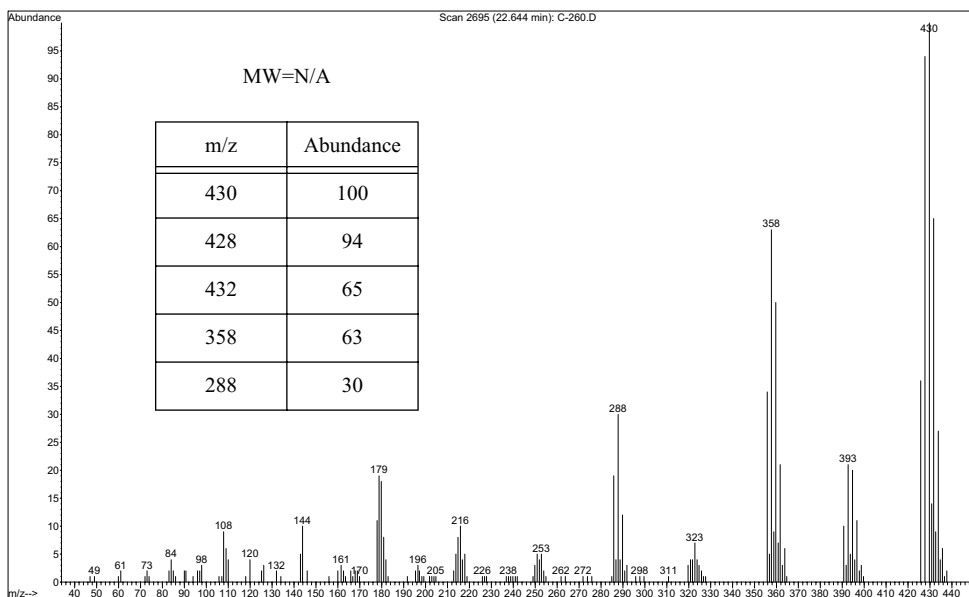
Used in electrical capacitors, electrical transformers, vacuum pumps, and gas-transmission turbines. Formerly used as heat transfer fluid, hydraulic fluids, rubber plasticizer, and in carbonless paper, adhesives, and wax extenders. Although the production and sale was discontinued in late 1977, it is still present in transformers and capacitors now in use.

Regulatory Information

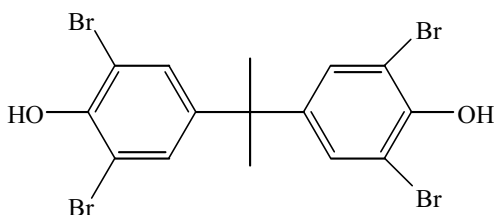
Section 6(e) of the Toxic Substances Control Act (TSCA) prohibits the manufacture, processing, and distribution in commerce of PCBs. In addition, the EPA has set a limit of 0.0005 mg of PCBs per liter of drinking water (0.0005 mg/L). Discharges, spills, or accidental releases of 1 lb or more of PCBs into the environment must be reported to the EPA. The Food and Drug Administration (FDA) requires that infant foods, eggs, milk and other dairy products, fish and shellfish, poultry, and red meat contain no more than 0.2 to 3 parts of PCBs per million parts (0.2 to 3 ppm) of food.

Toxicological and Environmental Data

PCBs do not readily break down in the environment and thus may remain there for very long periods of time. PCBs can travel long distances in the air and be deposited in areas far away from where they were released. In water, a small amount of PCBs may remain dissolved, but most stick to organic particles and bottom sediments. PCBs also bind strongly to soil. PCBs are taken up by small organisms and fish in water and accumulate up the food chain in fish and marine mammals.



For Chromatogram See Appendix A - C-260 - page 536

Firemaster BP4A**CAS Number** 79-94-7**RTECS Number** SM0894500**Abbreviation** TBBPA**Formula** C₁₅H₁₂Br₄O₂**Molecular Weight** 543.91**Chemical Name**

4,4'-(1-methylethylidene)bis(2,6-dibromophenol)

Synonyms

bromdian; Fireguard 2000; 2,2',6,6'-Tetrabromobisphenol A; 3,3',5,5'-Tetrabromobisphenol A; Tetrabromodiphenylopropane; Tetrabromodian

Application

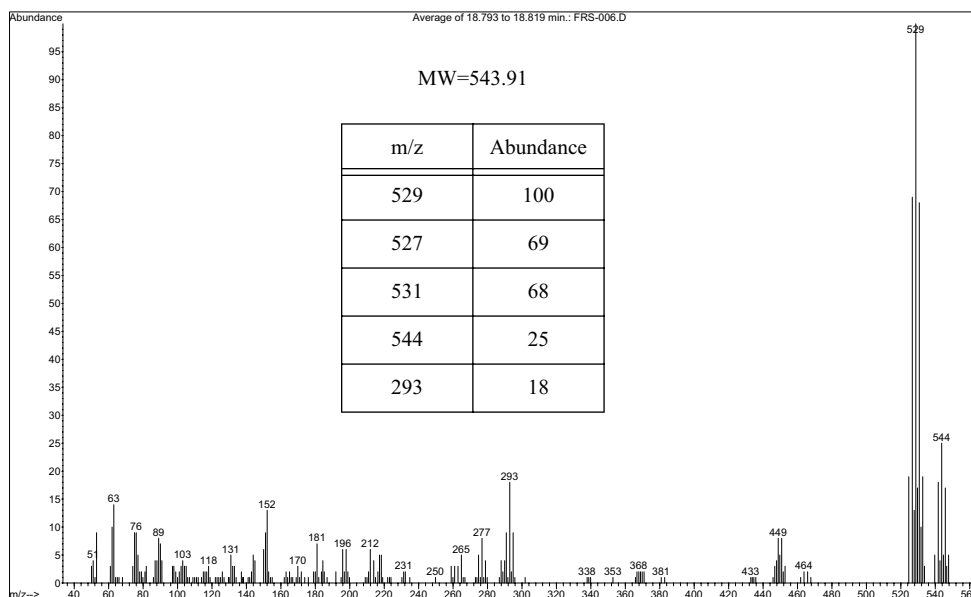
The primary use of TBBPA is as a flame retardant in epoxy resin circuit boards and in electronic enclosures made of polycarbonate-acrylonitrile-butadiene-styrene (PC-ABS). Other applications of TBBPA include its use as a flame retardant for plastics, paper, and textiles; as a plasticizer; in adhesives and coatings; and as a chemical intermediate for the synthesis of other flame retardants (e.g., TBBPA allyl ether). It has also been applied to carpeting and office furniture as a flame retardant.

Regulatory Information

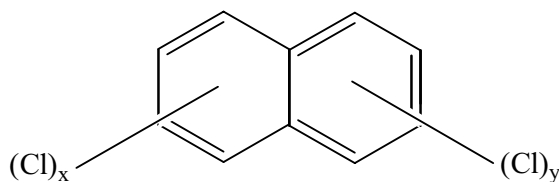
There are currently no legislative restrictions on the use of TBBPA.

Toxicological and Environmental Data

TBBPA enters waste streams from production of circuit boards and other applications and enters the environment via disposal of products containing TBBPA. RTECS CLASS OF COMPOUND: Reproductive effector; primary irritant. Lowest published toxic oral dose (TDLo): 250 mg/kg (6-15 d preg) [Rat].



For Chromatogram See Appendix A - FRS-006 - page 537

Halowax 1001**CAS Number** 58718-67-5**RTECS Number** N/A**Abbreviation** Not Identified**Formula** Technical mixture**Molecular Weight** ~255**Chemical Name**

polychlorinated naphthalene 1001

Synonyms

N/A

Application

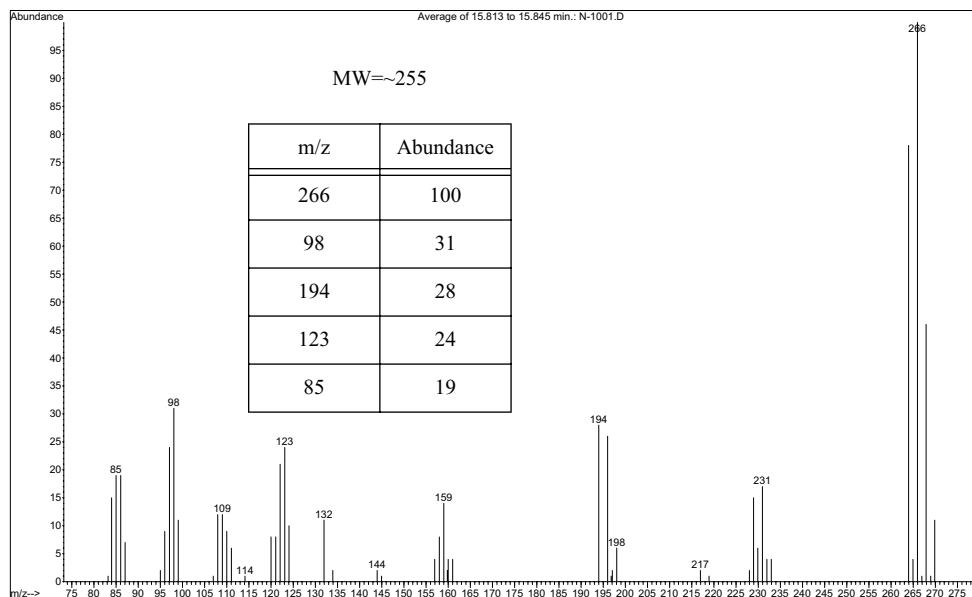
Used as paper impregnant in automobile capacitors (dielectrics). Electrical insulation and fire-resisting materials; impregnants; sealing compounds; crankcase additive; ingredient in penetrating oils; plasticizer; protective coatings.

Regulatory Information

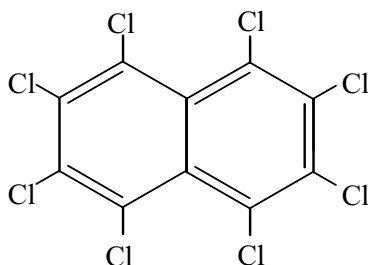
Regulated by the EPA under the Clean Water Act (CWA), and the Clean Air Act.

Toxicological and Environmental Data

Chlorinated naphthalenes (CN) are persistent environmental contaminants, which accumulate and biomagnify in human and wildlife food-chains. Many of the CN congeners show relatively high dioxin-like activity and have been identified as common food contaminants, especially in fish.



For Chromatogram See Appendix A - N-1001 - page 538

Halowax 1051**CAS Number** 2234-13-1**RTECS Number** QK0250000**Abbreviation** Not Identified**Formula** Technical mixture**Molecular Weight** 403.73**Chemical Name**

octachloronaphthalene

Synonyms

octachloronaphthalene; perchloronaphthalene; 1,2,3,4,5,6,7,8-octachloronaphthalene

Application

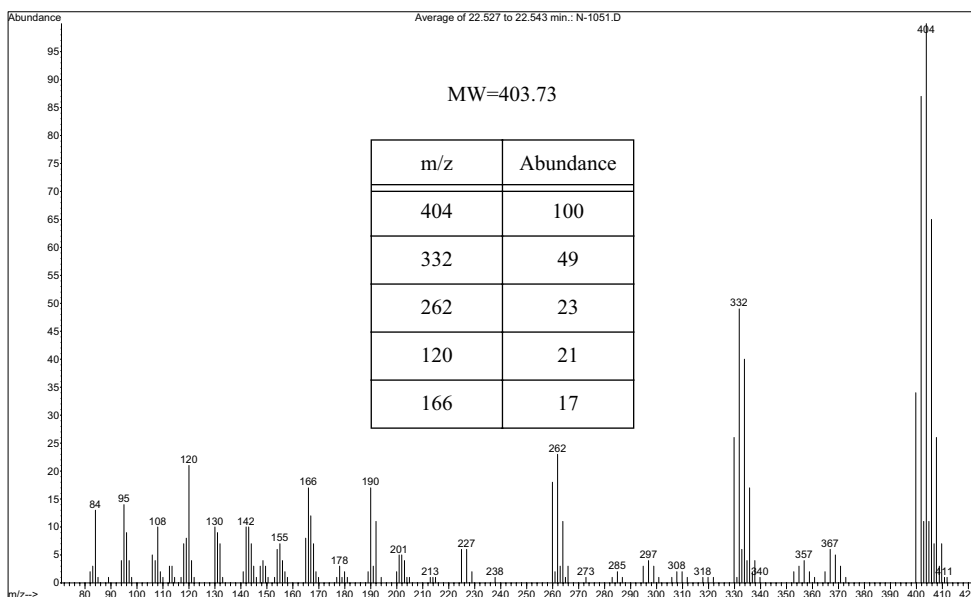
Insulating material in capacitors and cable manufacturing. Halowax 1051 is a technical mixture, the octachloronaphthalene is the primary and target component.

Regulatory Information

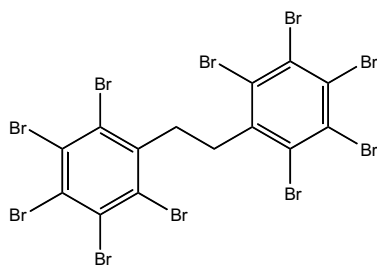
Regulated by the EPA under the Clean Water Act (CWA), CERCLA and the Clean Air Act.

Toxicological and Environmental Data

Chlorinated naphthalenes are persistent environmental contaminants, which accumulate and biomagnify in human and wild-life food-chains.



For Chromatogram See Appendix A - N-1051 - page 539

Saytex® 8010**CAS Number** 84852-53-9**RTECS Number** DA0358200**Abbreviation** DBDPE**Formula** C₁₄H₄Br₁₀**Molecular Weight** 971.22**Chemical Name**

1,2-bis(pentabromophenyl) ethane

Synonyms

ethane-1,2-bis(pentabromophenyl); decabromodiphenyl ethane

Application

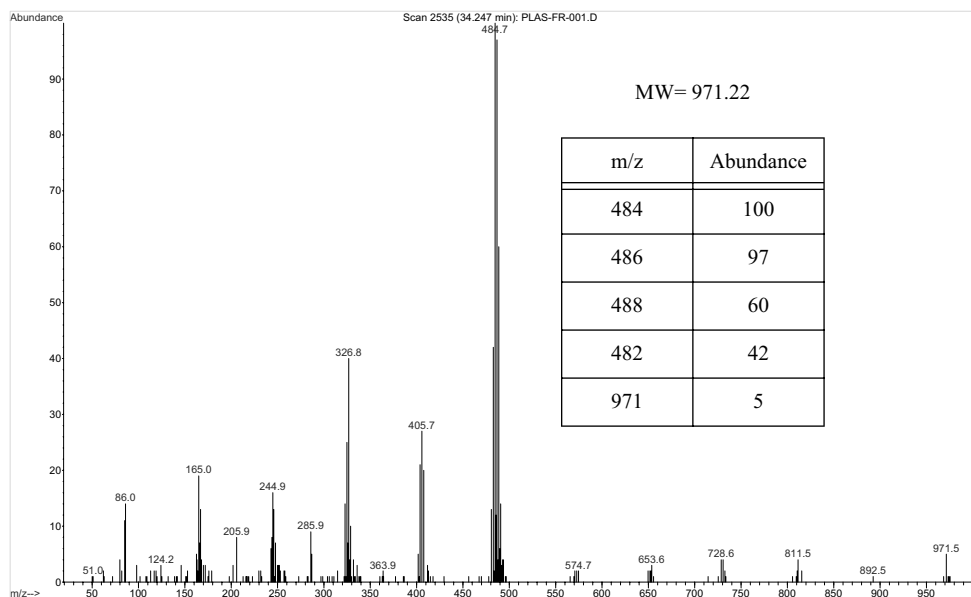
Flame retardant that can be used in a wide range of high performance applications such as styrenic polymers, engineering resins, wire and cable, and elastomers. Especially suitable for applications involving high temperature, a requirement for color stability, or where recycling is anticipated.

Regulatory Information

There is no information to indicate that the substance necessarily poses a risk, but rather that certain measures should be taken in the absence of sufficient information to make a decision.

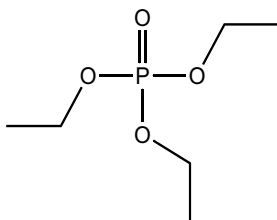
Toxicological and Environmental Data

The leaching potential from polymers is unknown, but is expected to be low in view of its very low water solubility and strong adsorption to organic carbon. Similarly, the low vapor pressure should limit its volatility. Emissions from landfills are therefore expected to be relatively small. This substance is poorly absorbed via the oral route. Based on physico-chemical properties, absorption following inhalation or dermal exposure is likely to be very low.



For Chromatogram See Appendix A - PLAS-FR-001 - page 540

Triethylphosphate



CAS Number 78-40-0

RTECS Number TC7900000

Abbreviation TEP

Formula $C_6H_{15}O_4P$

Molecular Weight 182.15

Chemical Name

triethyl phosphate

Synonyms

phosphoric acid, triethyl ester

Application

TEP is used as a flame retardant for making non-flammable polyurethane foams and polyurethane resins as well as a viscosity reducer for polyols and prepolymers.

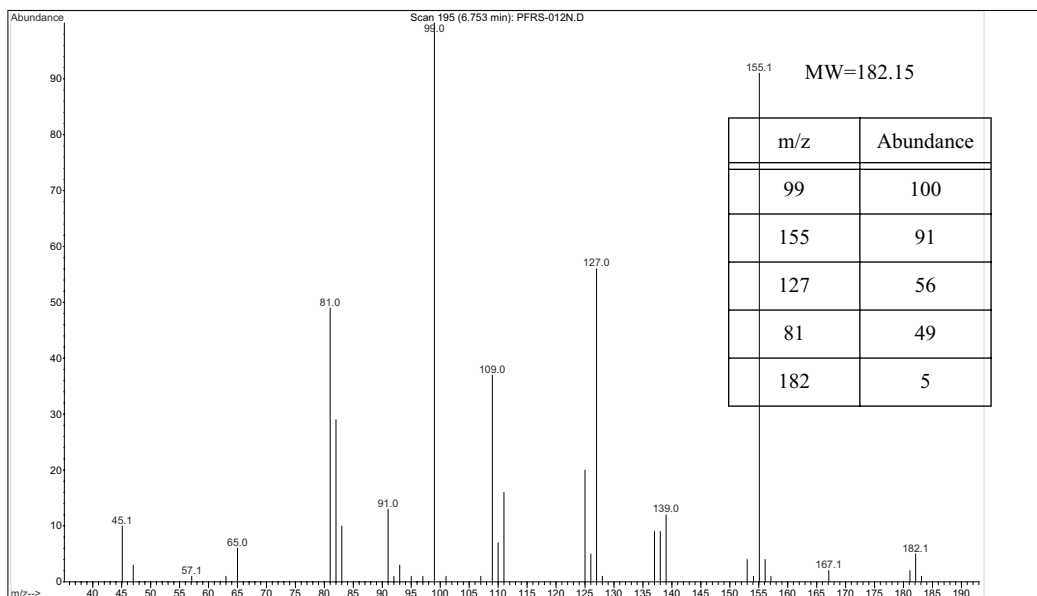
Regulatory Information

Not FDA approved for food contact applications.

Toxicological and Environmental Data

Oral (LD50): Acute: 1500 mg/kg [Mouse] : oral (LD50): 1600 mg/kg [Rat].

Classified as “inherently biodegradable” (with industrial inoculum) with a “low bioaccumulation potential.” The most sensitive environmental species to TEP is *Daphnia magna* (21d-NOEC = 31.6 mg/l).



For Chromatogram See Appendix A - PFRS-012 - page 541

Plasticizers

Plasticizers are one of the most important classes of polymer additives in the sense that the volume of application is very high and the applications are broad across a wide range of polymeric materials. These are the compounds that promote flexibility and durability in a wide range of polymers that would otherwise be hard, inflexible, and impact-sensitive. The highest volume of plasticizer use is for PVC, which is in turn used in a wide variety of compounds ranging from plumbing components, construction materials, automotive interiors, furniture, electrical insulation, and many others. In most cases, the plasticizer is not grafted to the polymer. As a result, these compounds can migrate to the surface of the finished plastic product and then evaporate or leach into the surrounding environment. This disadvantage for use is an advantage for analysis because these plasticizers are easily desorbed from the base polymer.

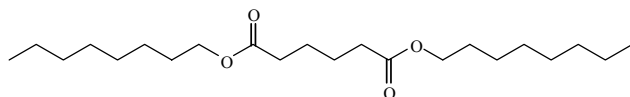
A wide variety of plasticizers are commercially available and novel types are replacing older compounds that were less stable or have higher environmental impact. Typical requirements for selection of a plasticizer include compatibility with the host polymer, low extractability by water and solvents, stability under heat and light exposure, good low-temperature properties, ease of processing, and low odor, taste, toxicity, and cost. Since no single plasticizer meets all of these requirements, and some are more appropriate than others for a specific polymer, blending of multiple plasticizers is often necessary to achieve the desired result in the final product.

The most commonly used plasticizers are phthalates. These include dioctyl phthalate, di(2-ethylhexyl) phthalate, diisodecyl phthalate, diisononyl phthalate, and a number of other phthalate esters. Concerns about possible carcinogenic effects have led to a steady decrease in the use of phthalates.

Epoxidized oils such as soybean, linseed, and tall oil fatty acids are also used as plasticizers. While they do not pose the same health risks as the phthalates, they have limited compatibility with PVC and cannot be used at high temperatures.

Adimoll DO

Lanxess

**CAS Number** 123-79-5**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₂H₄₂O₄**Molecular Weight** 370.57**Chemical Name**

hexanedioic acid, dioctyl ester

Synonyms

di-N-octyl adipate; dioctyl hexanedioate; bis(2-ethylhexyl) hexanedioate; dicaprylyl adipate; adipic acid, dioctyl ester

Brand Names & ManufacturersJayflex[®] DOA

ExxonMobil

Kodaflex[®] DOA

Eastman Chemical

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** -70.0 °C**Boiling Point** 215 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-80

Application, Regulatory & Environmental Information

Application Adimoll[®] DO is a low-temperature-resistant plasticizer suitable for a large number of polymers, for example, polyvinyl chloride (PVC), acrylonitrile-butadiene rubber (NBR), styrenebutadiene rubber (SBR), and polyvinyl acetate (PVAC). Commonly used in plastic wraps for food storage.

Regulatory Information

Adimoll DO can be used when regulations and recommendations governing food contact applications need to be met. The FDA has approved this material to be used to make plastic packaging as indirect food additives (substances which may come in contact with food as part of packaging or processing equipment but are not intended to be added directly to food).

Environmental Impact

If released into the environment, this material is expected to partition into the soil and sediment. It has a high potential to bioaccumulate. Not considered to be a source of air pollution.

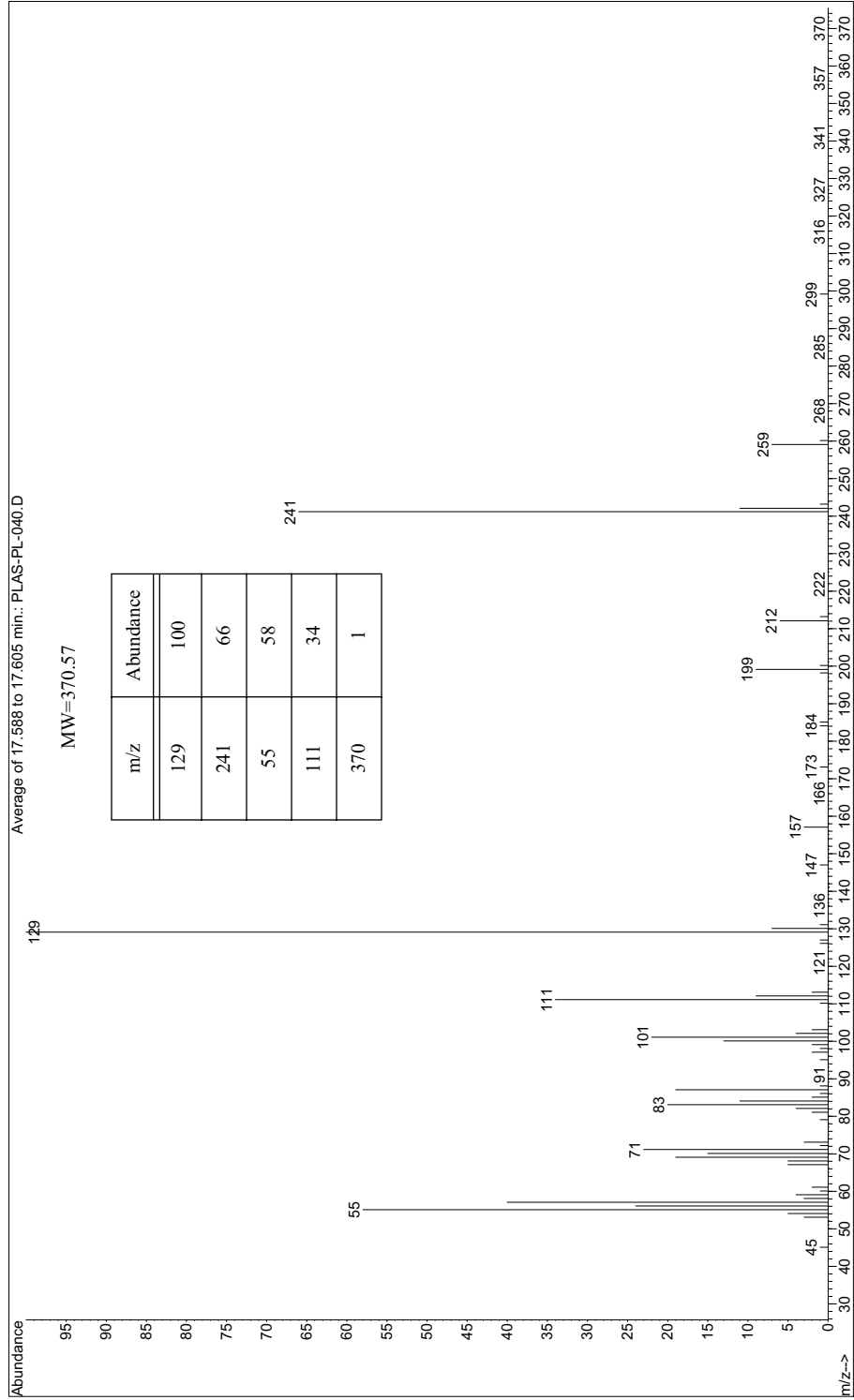
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products. Migrates into fatty foods with fat percentages >35%.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

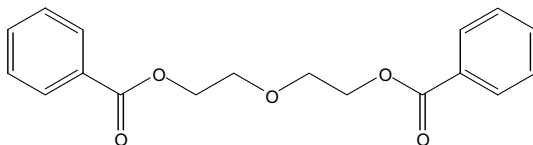
Mass Spectrum for Adimoll DO - PLAS-PL-040



For Chromatogram See Appendix A - PLAS-PL-040 - page 542

Benzoflex® 2-45

Velsicol Chemical Corporation

**CAS Number** 120-55-8**RTECS Number** ID6650000**Abbreviation** DEGDB**Formula** C₁₈H₁₈O₅**Molecular Weight** 314.33**Chemical Name**

diethylene glycol, dibenzoate

Synonyms

benzoic acid, diester with diethylene glycol; dibenzoyldiethyleneglycol ester; benzoyloxyethoxyethyl benzoate

Brand Names & Manufacturers

K-Flex® DE

Emerald Kalama Chemical, LLC

Physical Properties**Appearance** Liquid**Melting Point** 28 °C**Boiling Point** 236 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	1-10	1-10	1-10

Application *Application, Regulatory & Environmental Information*

Used as a plasticizing agent for cellulose acetate butyrate. Used in the production of food contact cellulose nitrate resins, ethyl cellulose resins, PMMA resins, and polyvinyl acetate.

Regulatory Information

FDA approved as a component of adhesives for use in contact with food, 21CFR175.105; a component of the uncoated or coated food surface of paper and paperboard intended for use in producing, manufacturing, packaging, processing, preparing, treating, packing, transporting, or holding dry, aqueous, and fatty foods, 21CFR176.170 and 21CFR176.180.

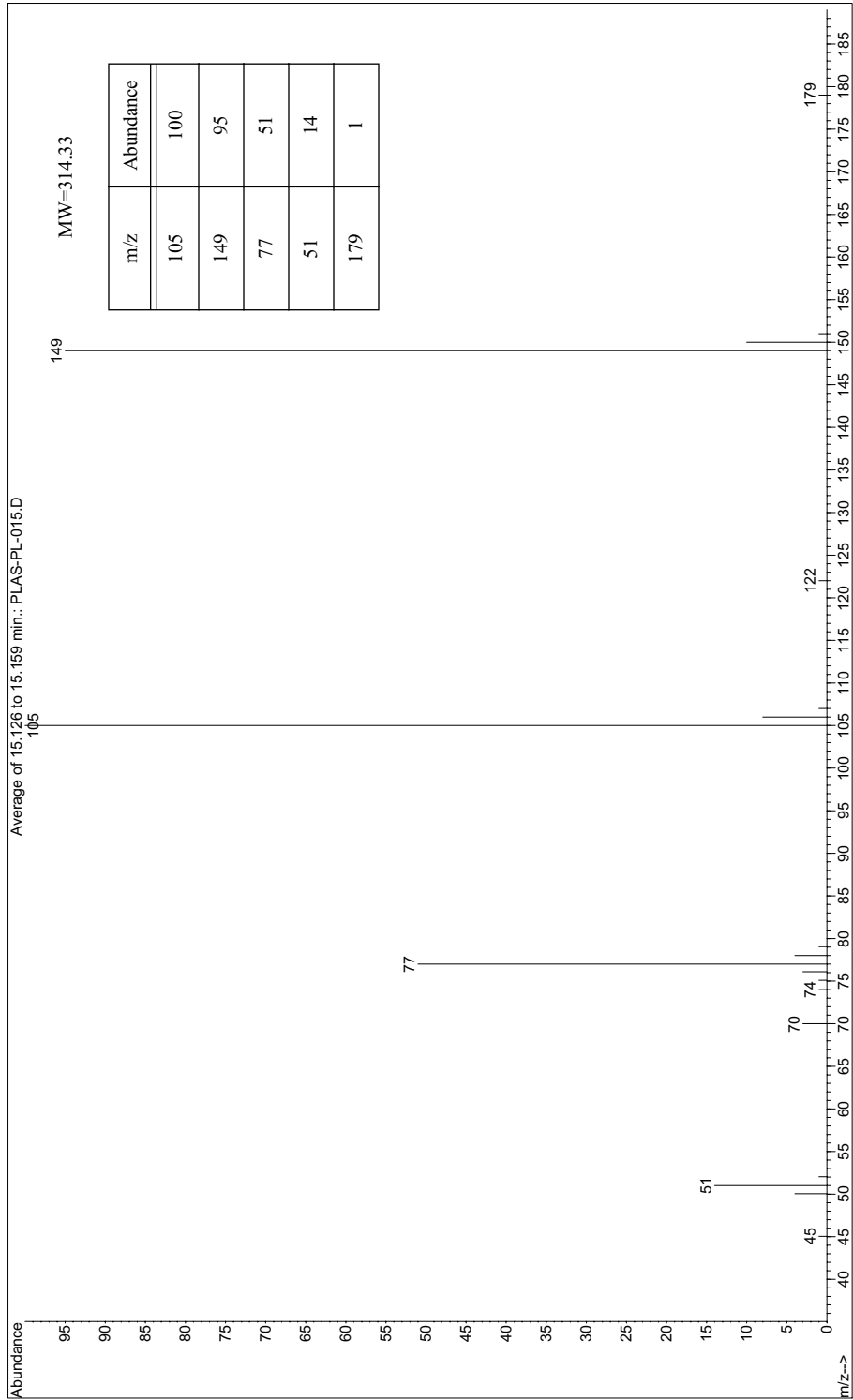
Environmental ImpactNo observed effect level: 1000 ppm, earthworm. (EC50): >10 mg/L, [Bacteria] (*Pseudomonas putida*); no inhibitory effect on the respiration rate of activated sludge at concentrations up to 100 mg/L. Considered ultimately biodegradable under anaerobic conditions in the biogas production test. European labeling: R52/53 — Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment; S61 — Avoid release to the environment.**Point of Release**

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

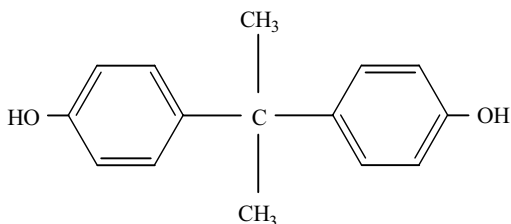
Toxicological Data

Decreased body weight gain and blood, spleen, and caecum effects were reported in rats given up to 2500 mg/kg/day DEGBD in their diet for 13 weeks. Acute dermal toxicity (LD50): 20 mL/kg [Rabbit]; acute oral (LD50): 2830 to 4190 mg/kg [Rat]; acute dermal (LD50): > 2000 mg/kg [Rat].

Mass Spectrum for Benzoflex® 2-45 - PLAS-PL-015



For Chromatogram See Appendix A - PLAS-PL-015 - page 543

Bisphenol A**CAS Number** 80-05-7**RTECS Number** SL6300000**Abbreviation** BPA**Formula** C₁₅H₁₆O₂**Molecular Weight** 228.29**Chemical Name**

4,4'-dihydroxy-2,2-diphenylpropane

Synonyms

4,4'-(propan-2-ylidene)diphenol; p,p'-isopropylidenebisphenol; 2,2-bis(4-hydroxyphenyl)propane

Brand Names & Manufacturers

Sold as bulk chemical

Varied

Physical Properties**Appearance** White to light brown flakes or powder**Melting Point** 157 °C**Boiling Point** 220 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Originally synthesized in 1891 and was investigated in the 1930s as a possible synthetic estrogen. Currently, the primary use is in the manufacture of polycarbonate plastics and epoxy resins for coatings on metal cans to maintain the quality of canned food and beverages. Also used as a thermal stabilizer in PVC compounds and as a dental sealant.

Regulatory Information

FDA has approved the use of Bisphenol A as a component used to make polyarylate or 4,4'-isopropylidenediphenol-epichlorohydrin resins to be used for single and repeated use food contact surfaces as outlined in 21CFR177, Parts 1440 and 1555. OSHA PEL in Shipyards ceiling concentration 0.5 ppm (2.8 mg/m³).

Environmental Impact

Real world monitoring studies show that BPA is rapidly biodegraded and extensively removed in wastewater treatment systems. Studies using real world surface water samples taken from various geographies demonstrate rapid degradation with a half-life in the range of 1 to 4 days. Bisphenol A does not accumulate in aquatic organisms to any appreciable extent and is not classified as bioaccumulative by the USEPA.

Point of Release

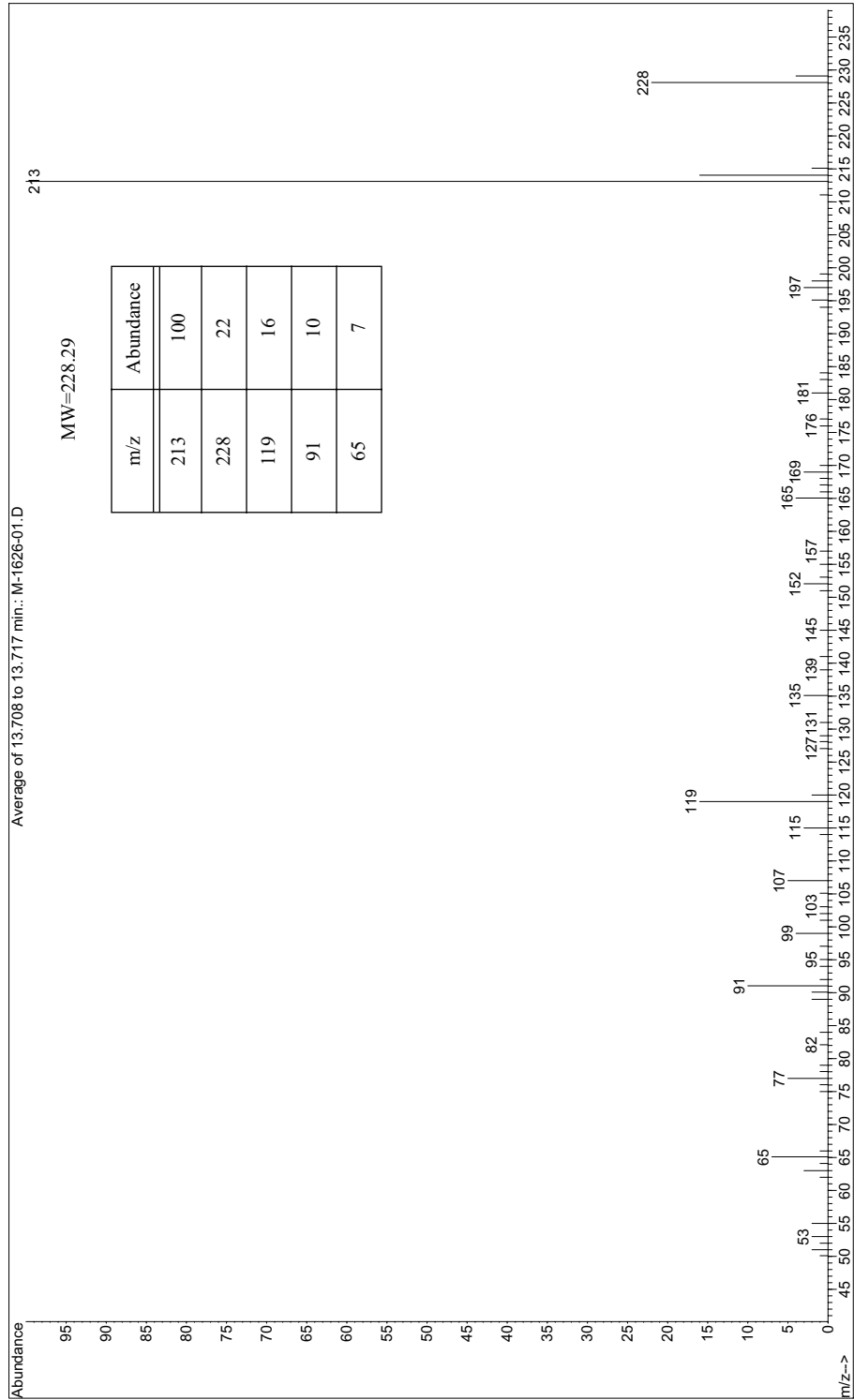
Low levels may be released to the environment in the effluent water from biological wastewater treatment plants. Scientists have known for many years that the polycarbonate bond created by BPA is unstable and that the chemical will eventually leach into food or beverages in contact with the plastic. The obvious concern today is that it may leach into food products, ranging from microwavable dinners to baby formula, that are packaged in polycarbonate plastic.

Toxicological Data

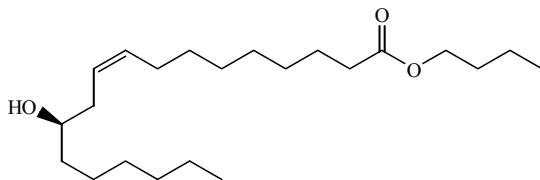
RTECS CLASS OF COMPOUND: tumorigen; hormone; mutagen; human data; primary irritant; reproductive effector.

Acute oral toxicity (LD50): 3250 mg/kg [Rat]; acute dermal toxicity (LD50): 3 mL/kg [Rabbit]; lowest published toxic oral dose (TDLo): 1000 mg/kg [Rat].

Mass Spectrum for Bisphenol A - M-1626-01



For Chromatogram See Appendix A - M-1626-01 - page 544

Butyl ricinoleate**CAS Number** 151-13-3**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₂H₄₂O₃**Molecular Weight** 354.57**Chemical Name**

12-hydroxy-9-octadecenoic acid, butyl ester

Synonyms

butyl ricinoleate; ricinolic acid butyl ester

Brand Names & Manufacturers

Flexricin® P-3

G.R. O'Shea/Vertellus

Physical Properties**Appearance** Yellow to colorless liquid**Melting Point** -26 °C**Boiling Point** 275 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information

Application Butyl ricinoleate is a plasticizer for polyvinyl butyral, rosin, vinsol resin, and cellulose acetate butyrate resins. Can also be used as a general purpose plasticizer for both nitrocellulose and ethylcellulose.

Regulatory Information

FDA approval under Section 175.105 for use in adhesives with indirect food contact.

Environmental Impact

This chemical is expected to readily biodegrade. If released into the environment it is expected to partition to sediment.

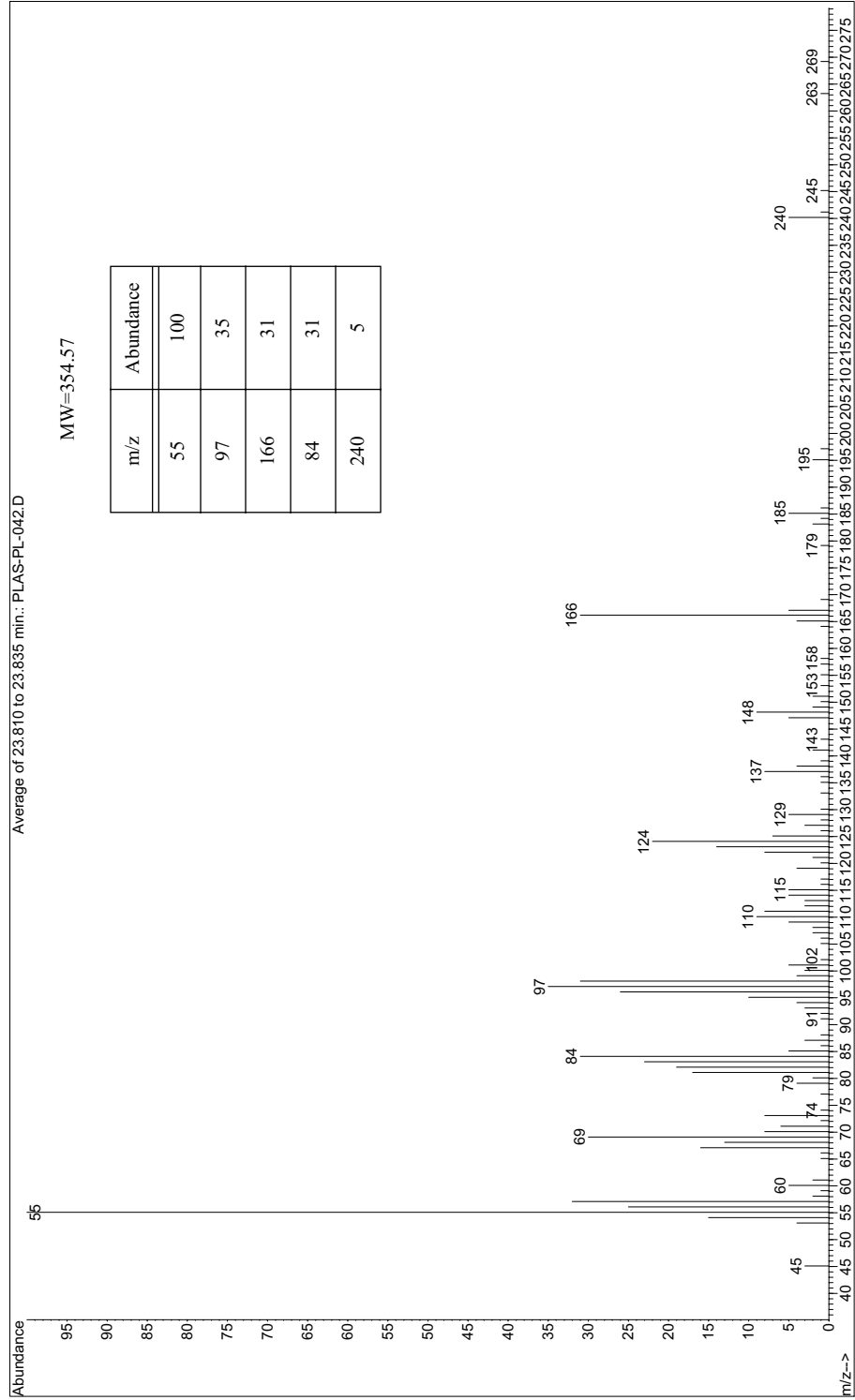
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

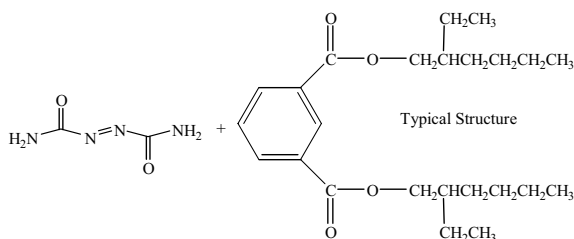
Mass Spectrum for Butyl ricinoleate - PLAS-PL-042



For Chromatogram See Appendix A - PLAS-PL-042 - page 545

Celogen® SD-125

Chemtura Corporation

**CAS Number** N/A**RTECS Number** N/A**Abbreviation** Not Identified**Formula** N/A**Molecular Weight** N/A**Chemical Name**

50% azodicarbonamide in a phthalate plasticizer

Synonyms

N/A

Brand Names & Manufacturers

Celogen SD-125

Chemtura Corporation

Physical Properties**Appearance** Viscous, yellow liquid**Melting Point** 190-220°C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1

Application, Regulatory & Environmental Information

Application Celogen® SD dispersions eliminate dust, improve dispersability in PVC plastisols, and may be metered directly into the manufacturing process. May be found in sponge rubber and expanded plastics.

Regulatory Information

FDA approved under 21CFR175.300 — Resinous and Polymeric Coatings, limited to can end cement, 177.1210 — Closures with Sealing Gaskets for Food Containers (limitation — 2% Max.), and 177.2600 — Rubber Articles Intended for Repeated Use (limitation — 5% Max.).

Environmental Impact

Degradation of azodicarbonamide by sewage sludge organisms has been investigated in three modified Sturm tests. The compound was “readily biodegradable” in two out of the three tests and was degraded by 21% over 30 days in the third test. According to Mackay Level I fugacity modelling, azodicarbonamide released to surface waters will partition to the hydro-sphere with no significant sorption to particulates.

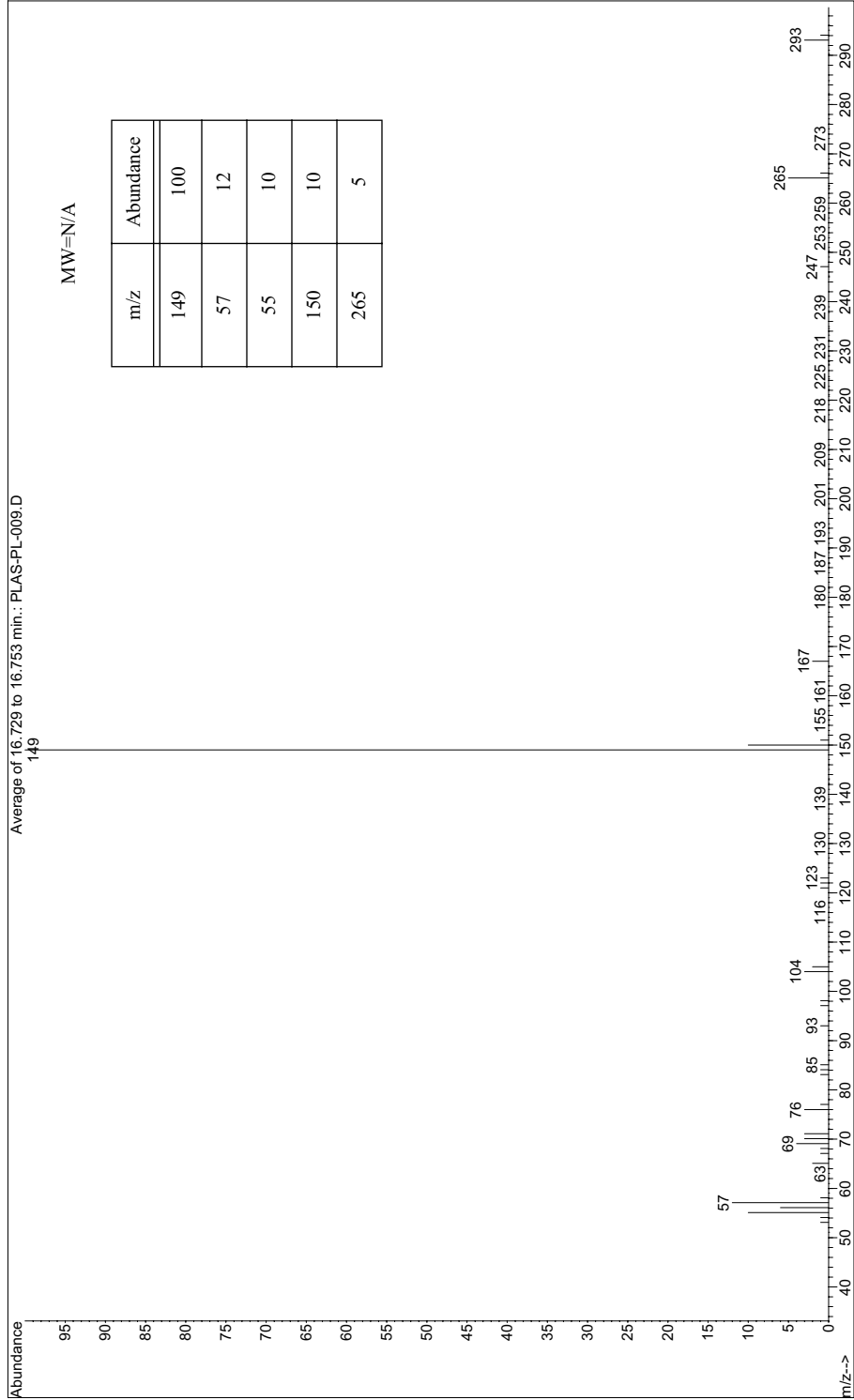
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

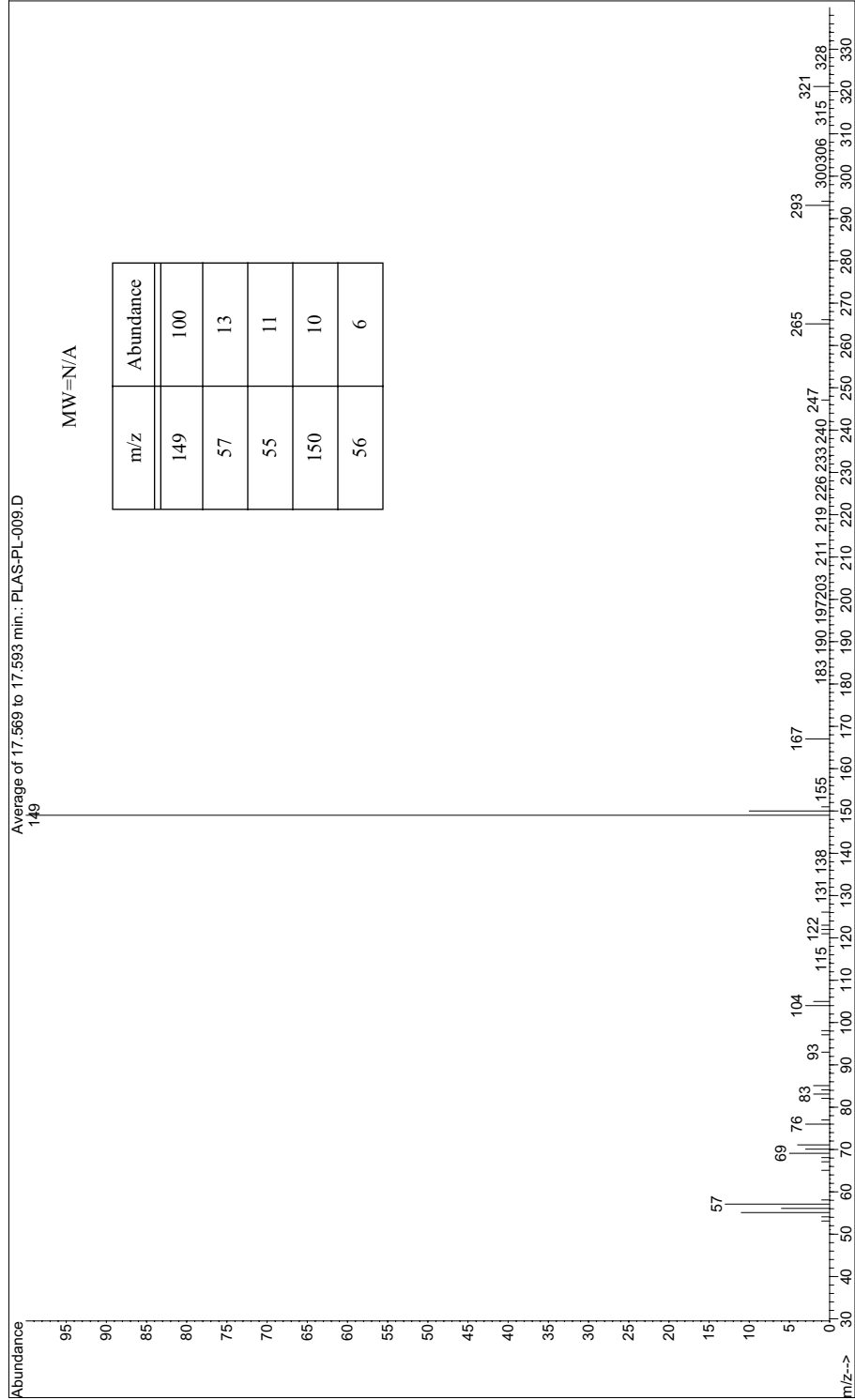
Studies in humans have concentrated solely on the ability of azodicarbonamide to induce asthma and skin sensitization. Evidence that azodicarbonamide can induce asthma in humans has been found from bronchial challenge studies with symptomatic individuals and from health evaluations of employees at workplaces where azodicarbonamide is manufactured or used. There are also indications that azodicarbonamide may induce skin sensitization.

Mass Spectrum for Celogen® SD-125 - PLAS-PL-009



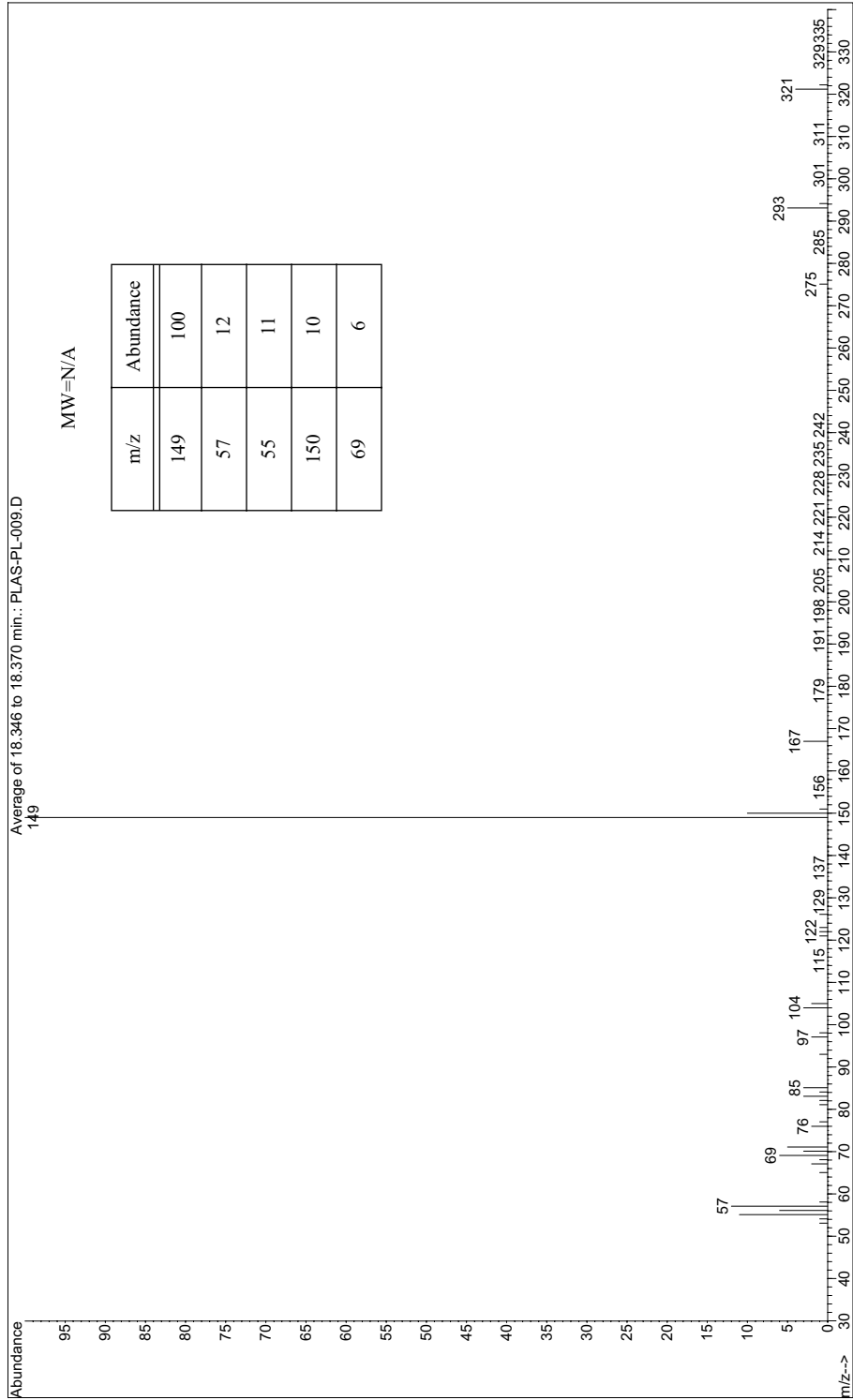
For Chromatogram See Appendix A - PLAS-PL-009 - page 546

Mass Spectrum for Celogen® SD-125 - PLAS-PL-009



For Chromatogram See Appendix A - PLAS-PL-009 - page 546

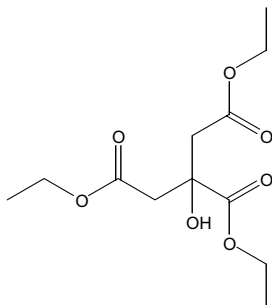
Mass Spectrum for Celogen® SD-125 - PLAS-PL-009



For Chromatogram See Appendix A - PLAS-PL-009 - page 546

Citroflex® 2

Morflex, Inc.

**CAS Number** 77-93-0**RTECS Number** GE8050000**Abbreviation** TEC**Formula** C₁₂H₂₀O₇**Molecular Weight** 276.32**Chemical Name**

2-hydroxy-1,2,3-propanetricarboxylic acid, triethyl ester

Synonyms

citric acid, triethyl ester; triethyl citrate

Brand Names & Manufacturers

Citroflex 2

Morflex, Inc.

Physical Properties**Appearance** Colorless liquid**Melting Point** -46.00 °C**Boiling Point** 127.00 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water 5.5	MeOH U	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane U
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Application *Application, Regulatory & Environmental Information*

TEC is used as a plasticizer that does not support fungal growth for cellulose derivatives (e.g., cellulose citrate), and polyvinyl acetate, as well as natural resins such as dammar and ester gums. It is also used as a fixing agent in perfumes and as a film strengthening agent in hair sprays and nail polish, and as an active ingredient in deodorants.

Regulatory Information

FDA approved 1998 for manufacturing of resinous and polymeric coatings for food-contact surface articles 21CFR175.300 and as a plasticizer in resinous and polymeric coatings for polyolefin films used in food-contact surface articles 21CFR175.320 for producing, manufacturing, packing, processing, preparing, treating, packaging, transporting, or holding food. EU approved 1995 as a food additive in dried egg whites. Joint FAO/WHO committee on Food Additives (1989) recommends ADI (Man): 10 mg/kg BW.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOCs), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

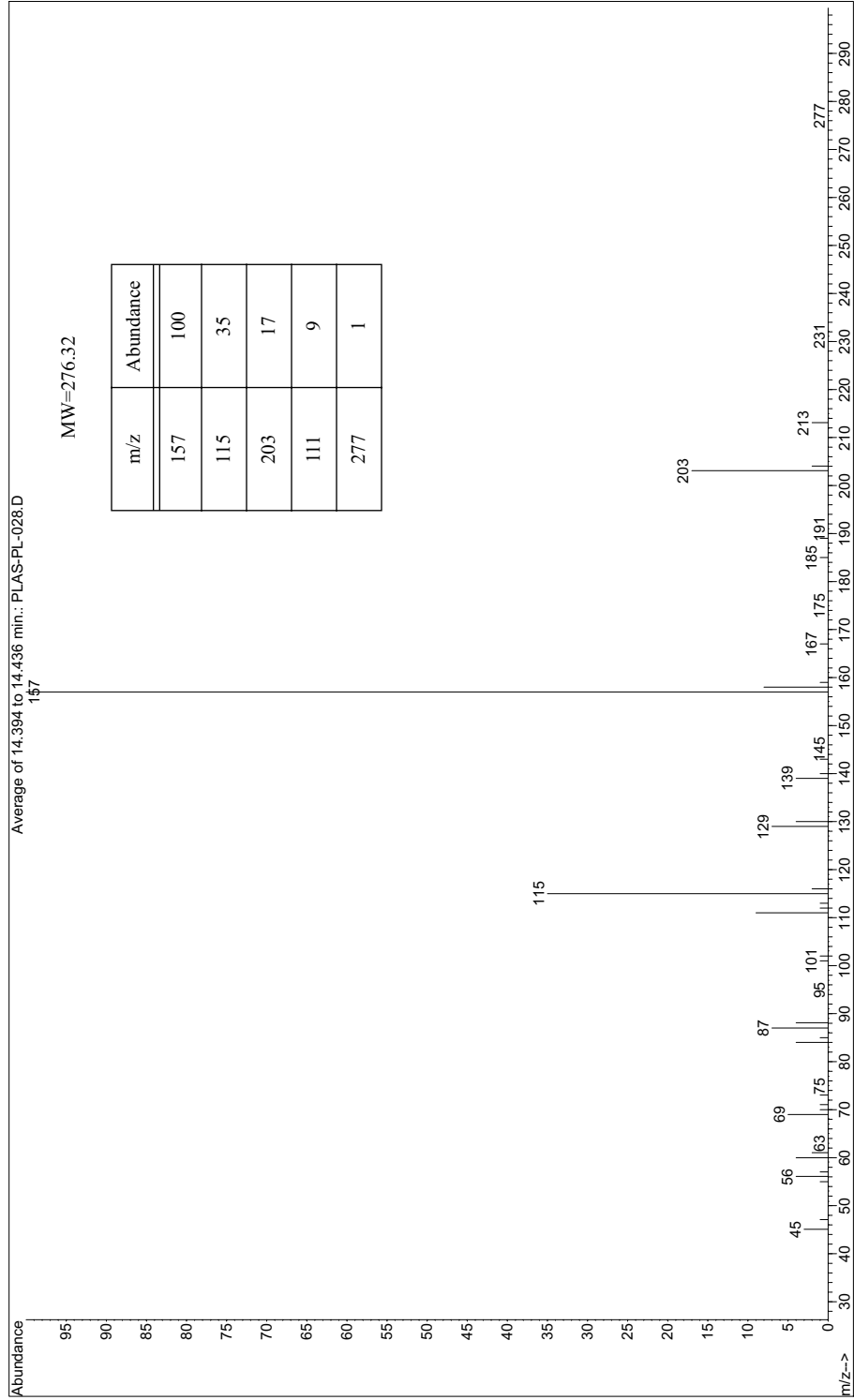
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Toxic action of TEC may occur due to calcium binding in bodily fluids and a reduction of blood pressure. Acute oral toxicity (LD50): 5900 mg/kg [Rat], acute inhalation toxicity (LD50): 1300 ppm/6 hour [Rat], acute dermal toxicity (LD50): >5 g/kg [Rabbit].

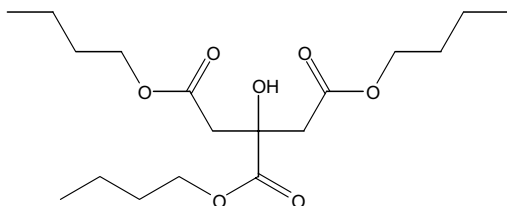
Mass Spectrum for Citroflex® 2 - PLAS-PL-028



For Chromatogram See Appendix A - PLAS-PL-028 - page 547

Citroflex® 4

Morflex, Inc.

**CAS Number** 77-94-1**RTECS Number** TZ8608000**Abbreviation** TBC**Formula** C₁₈H₃₂O₇**Molecular Weight** 360.45**Chemical Name**

2 hydroxy-1,2,3-propanetricarboxylic acid, tributyl ester

Synonyms

butyl citrate; citric acid, tributyl ester; tributyl 2-hydroxy-1,2,3-propanetricarboxylate

Brand Names & Manufacturers

Citroflex 4

Morflex, Inc.

Physical Properties**Appearance** Clear, colorless, viscous liquid**Melting Point** N/A**Boiling Point** 322 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂ U	Hexane
	<0.1	40-80	40-80	40-80		40-80

Application, Regulatory & Environmental Information

Application TBC is used as a plasticizer that does not support fungal growth in cellulosic and vinyl resins (especially PVC), polyactic acid resins (as a biodegradable component), and furniture coatings. Also used as a solvent for nitrocellulose and lacquers intended for food contact applications. Additional applications include a defoaming agent in proteinaceous solutions.

Regulatory Information

FDA approved 1998 as a component of food contact adhesives to be used safely as a component of articles intended for use in packaging, transporting, or holding food, 21CFR175.105.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOCs), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

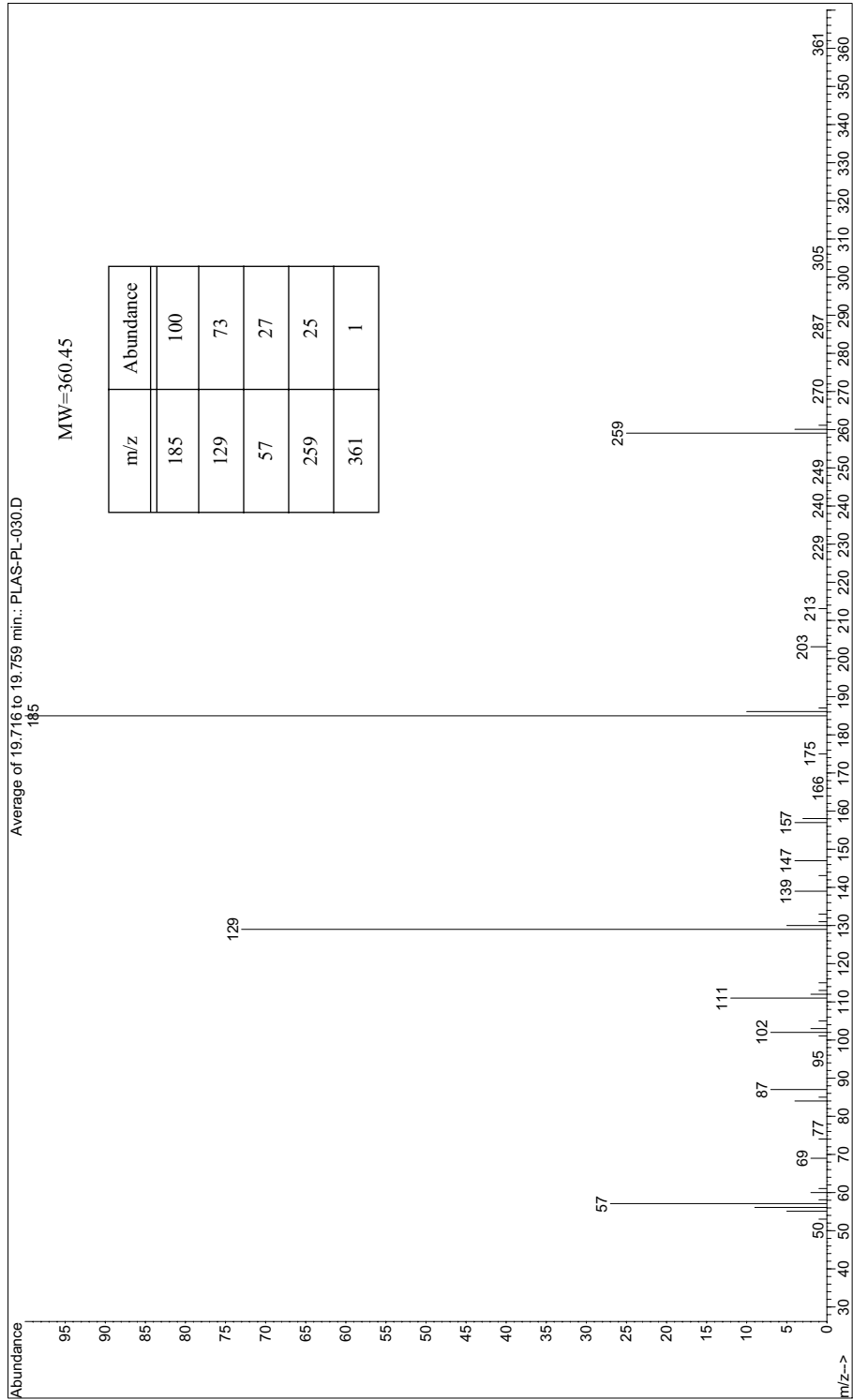
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Insoluble in body fluids resulting in low toxicity. Single dose of 10 to 30 mL/kg BW does not result in intoxication.

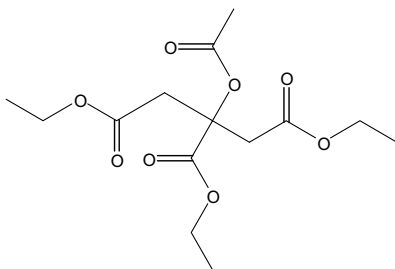
Mass Spectrum for Citroflex® 4 - PLAS-PL-030



For Chromatogram See Appendix A - PLAS-PL-030 - page 548

Citroflex® A-2

Morflex, Inc.

**CAS Number** 77-89-4**RTECS Number** GE8225000**Abbreviation** ATEC**Formula** C₁₄H₂₂O₈**Molecular Weight** 318.32**Chemical Name**

2-(acetyloxy)-1,2,3-propanetricarboxylic acid, triethyl ester

Synonyms

acetyltriethyl citrate; triethyl acetylcitrate

Brand Names & Manufacturers

Citroflex A-2

Morflex, Inc.

Physical Properties**Appearance** Clear liquid**Melting Point** Not available**Boiling Point** 228-229 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂ U	Hexane
	0.7	40-80	40-80	40-80		40-80

Application, Regulatory & Environmental Information

Application Citroflex® A-2 is used as a plasticizer in food-packing materials. Additional applications include use as a fixative for perfumes, a film strengthening agent in hair sprays, nail polish, and as a component in ink formulations.

Regulatory Information

FDA approved 1998 for the following applications: as a plasticizer in food-packaging materials, 21CFR178.3740; in adhesives as a component of articles intended for use in packaging, transporting, or holding food, 21CFR175.105; in the manufacture of resinous or polymeric coatings for the food-contact surface of articles intended for use in producing, manufacturing, packing, processing, preparing, treating, packaging, transporting, or holding food, 21CFR175.300; for use in the manufacture of resinous and polymeric coatings for polyolefin films, regulated under 21CFR175.320.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOCs), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

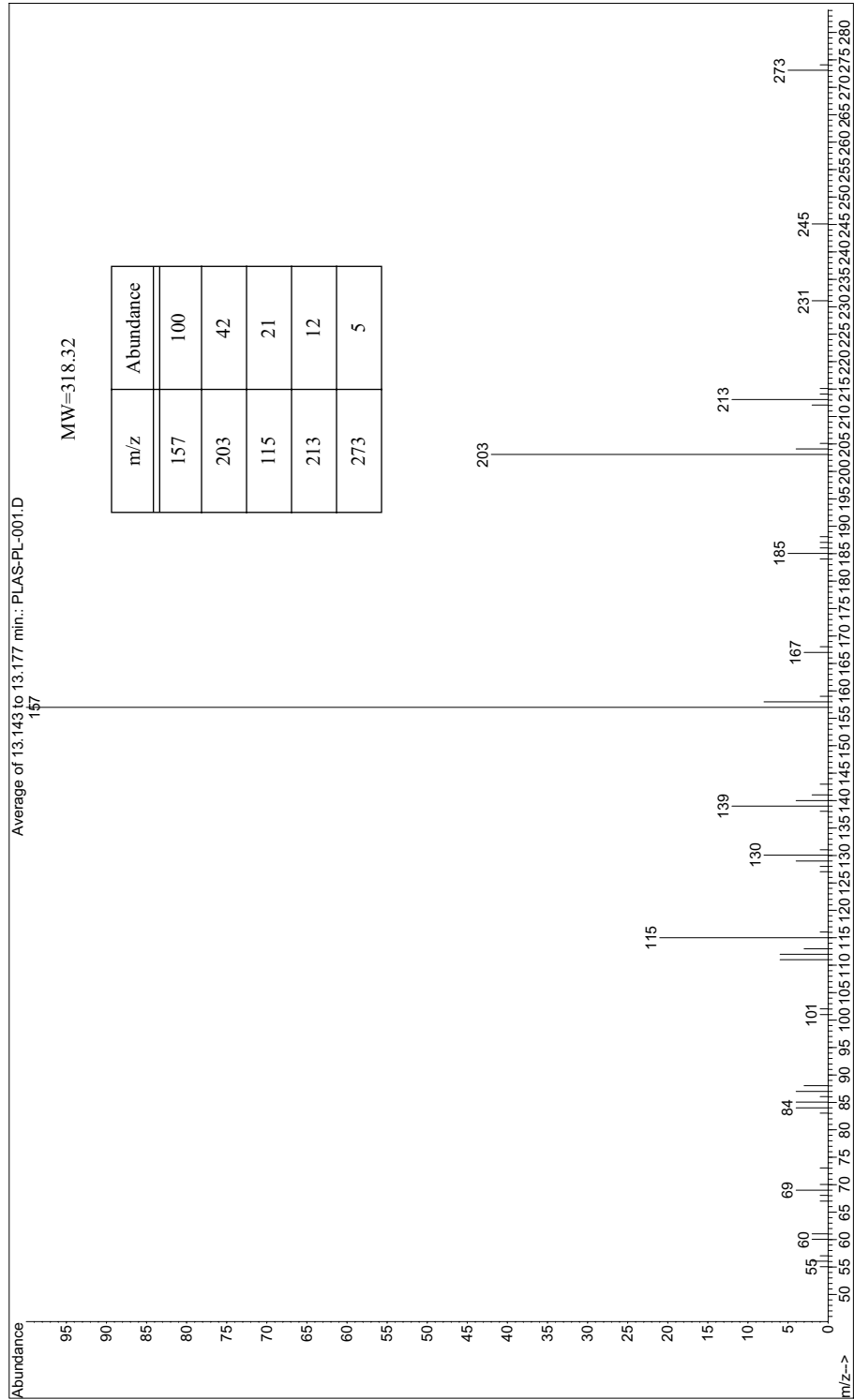
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute toxicity: (LD50): 7.0 g/kg BW [Rat].

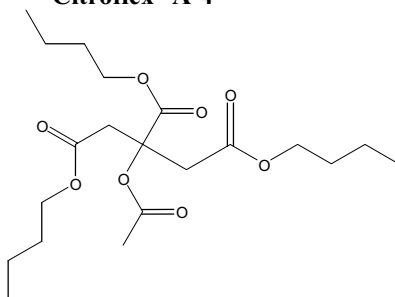
Mass Spectrum for Citroflex® A-2 - PLAS-PL-001



For Chromatogram See Appendix A - PLAS-PL-001 - page 549

Citroflex® A-4

Morflex, Inc.

**CAS Number** 77-90-7**RTECS Number** TZ8330000**Abbreviation** ATBC**Formula** C₂₀H₃₄O₈**Molecular Weight** 402.54**Chemical Name**

2-acetoxy-1,2,3-propanetricarboxylic acid, tributyl ester

Synonyms

acetyltri-n-butyl citrate; acetylcitric acid; acetyl tributyl citrate

Brand Names & Manufacturers

Citroflex A-4

Morflex, Inc.

Physical Properties**Appearance** Clear liquid**Melting Point** N/A**Boiling Point** 326 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂ U	Hexane
	<0.1	40-80	40-80	40-80		40-80

Application *Application, Regulatory & Environmental Information*

ATBC is used as a plasticizer for flexible films made of vinylchloride-vinylidene chloride copolymer and cellulose. It is used as a plasticizer in food contact applications and in vinyl toys for children (low toxicity). ATBC provides adherence to metals, low volatility, and resistance to yellowing. Also used in ink formulations, vinyl gloves, a non-VOC solvent in nitro-cellulose propellants, a plasticizer in nail polishes, adhesives, and coatings, and for coating both paperboard and foil.

Regulatory Information

FDA approved 1998 as a plasticizer in food-packaging materials, 21CFR178.3740; in adhesives as a component of articles intended for use in packaging, transporting, or holding food, 21CFR175.105; in the manufacture of resinous and polymeric coatings for safe use as a food-contact surface of articles, 21 CFR175.300; in the manufacture of resinous or polymeric coatings in polyolefin films for the food-contact surface of articles intended for use in producing, manufacturing, packing, processing, preparing, treating, packaging, transporting, or holding food, 21CFR175.320.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOCs), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

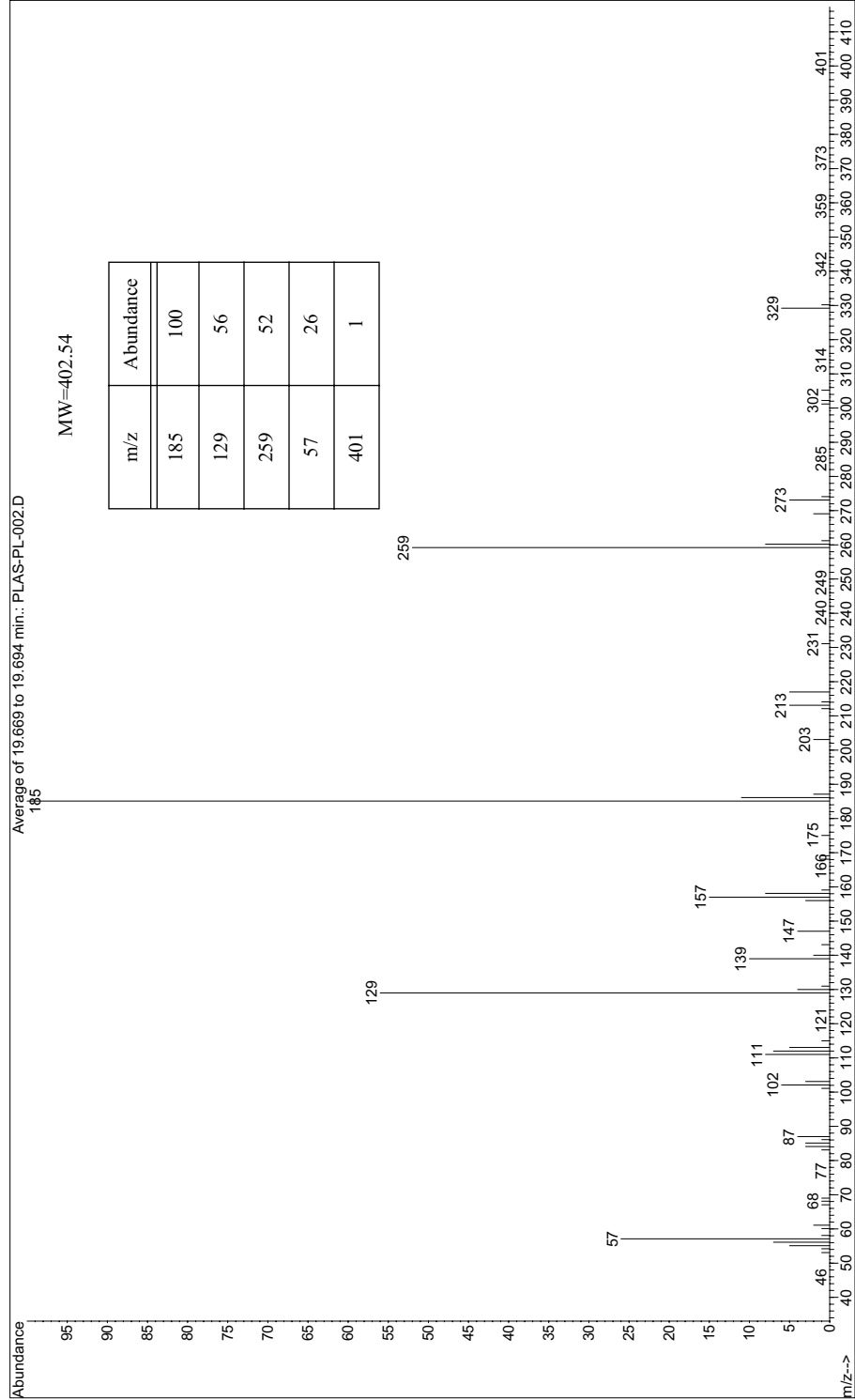
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): 31400 mg/kg [Rat], acute intraperitoneal toxicity (LD50): >4 gm/kg [Mouse].

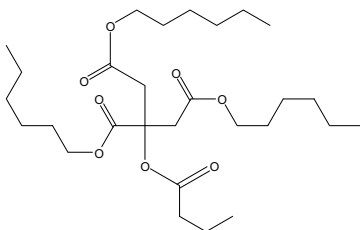
Mass Spectrum for Citroflex® A-4 - PLAS-PL-002



For Chromatogram See Appendix A - PLAS-PL-002 - page 550

Citroflex® B-6

Morflex, Inc.

**CAS Number** 82469-79-2**RTECS Number** N/A**Abbreviation** BTHC**Formula** C₂₈H₅₀O₈**Molecular Weight** 514.70**Chemical Name**

n-butyltri-n-hexyl citrate

Synonyms

2-(1-oxobutoxy)-1,2,3-propanetricarboxylic acid, trihexyl ester; butyrylcitric acid, tri-n-hexyl ester

Brand Names & Manufacturers

Citroflex B-6

Morflex, Inc.

Physical Properties**Appearance** Colorless to yellow, clear, oily liquid**Melting Point** -55 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	40-80	40-80	U	U

Application, Regulatory & Environmental Information

Application Specifically designed for use in medical articles especially blood storage bags. Considered to be an effective replacement for DEHP (di-2-ethylhexyl) phthalate and DEHA (di-2-ethylhexyl) adipate.

Regulatory Information

Citroflex B-6 is a component of several FDA approved blood bag systems, has a Drug Master File and is manufactured under Current Good Manufacturing Practice (CGMP) guidelines.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOCs), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

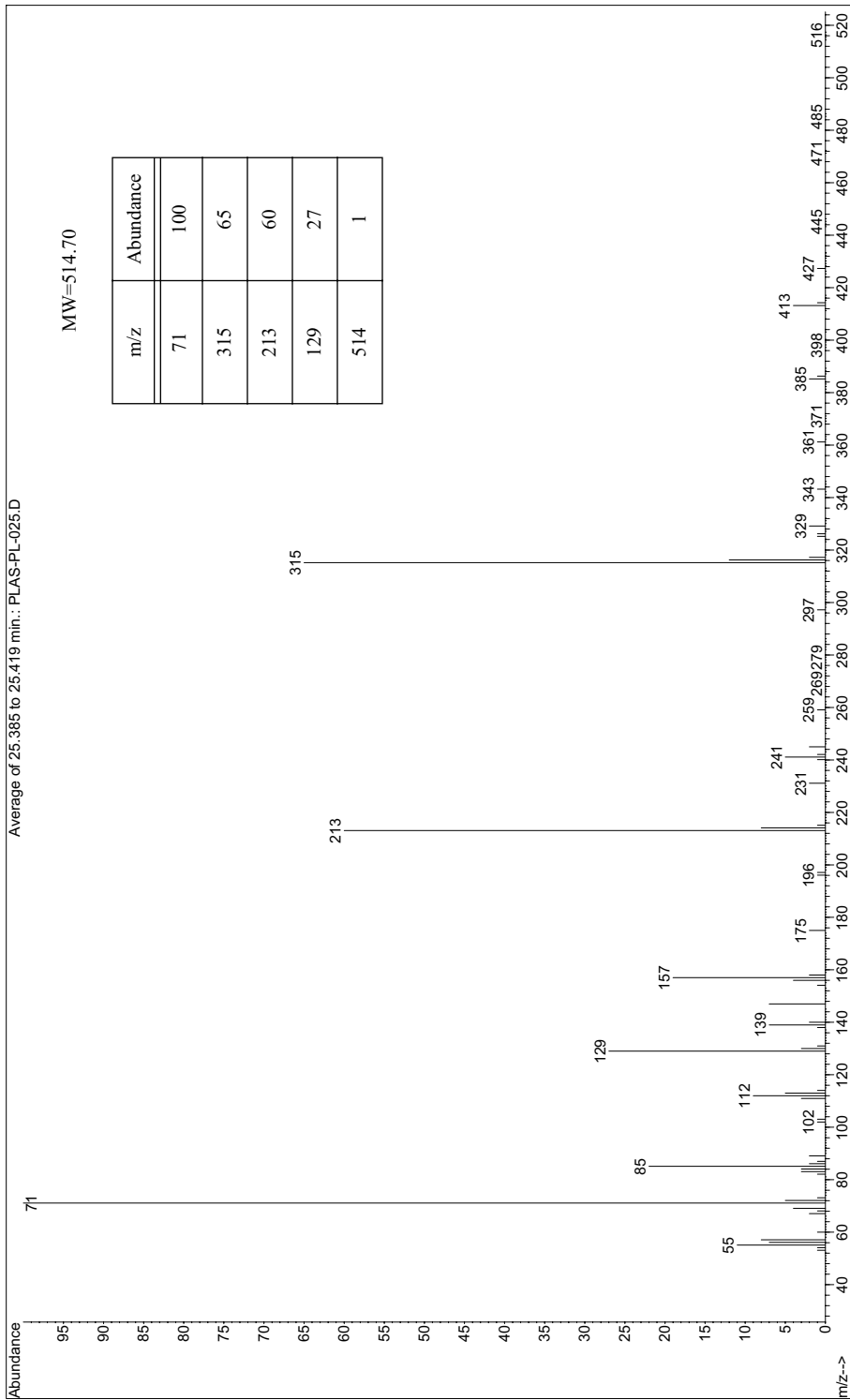
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

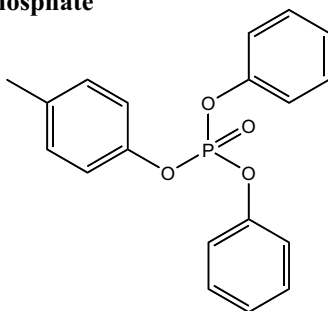
Toxicological Data

Acute oral toxicity (LD50): >20,000 mg/kg [Rat]. Rats fed this material showed no more abnormalities than those in the control group.

Mass Spectrum for Citroflex® B-6 - PLAS-PL-025



For Chromatogram See Appendix A - PLAS-PL-025 - page 551

Cresyl Diphenyl Phosphate**CAS Number** 26444-49-5**RTECS Number** TC5520000**Abbreviation** CDP**Formula** C₁₉H₁₇O₄P**Molecular Weight** 340.31**Chemical Name**

(4-methylphenyl) diphenyl phosphate

Synonyms

diphenyl cresol phosphate; phosphoric acid methylphenyl diphenyl ester

Brand Names & Manufacturers

Disflamoll® DPK

Lanxess

Phosflex® 112

Santicizer® 140

Physical Properties**Appearance** Clear liquid**Melting Point** -38 °C**Boiling Point** 235-255 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.0026	U	U	U	U	U

Application, Regulatory & Environmental Information**Application** Used as a plasticizer and flame retardant in the production of PVC, PS, PC, butadiene rubber, cellulose acetate, and aceto-butylate.**Regulatory Information**

FDA regulated for use as an indirect food additive — 21CFR §175.105 (adhesive components)

Environmental Impact

Readily biodegradable. 75%/28 d.

Calculated fugacity level III. 100% to water: In air = 0%, in water = 97.6%, in sediment = 2.3%, in soil = 0.1%.

Potential for bioaccumulation is high.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

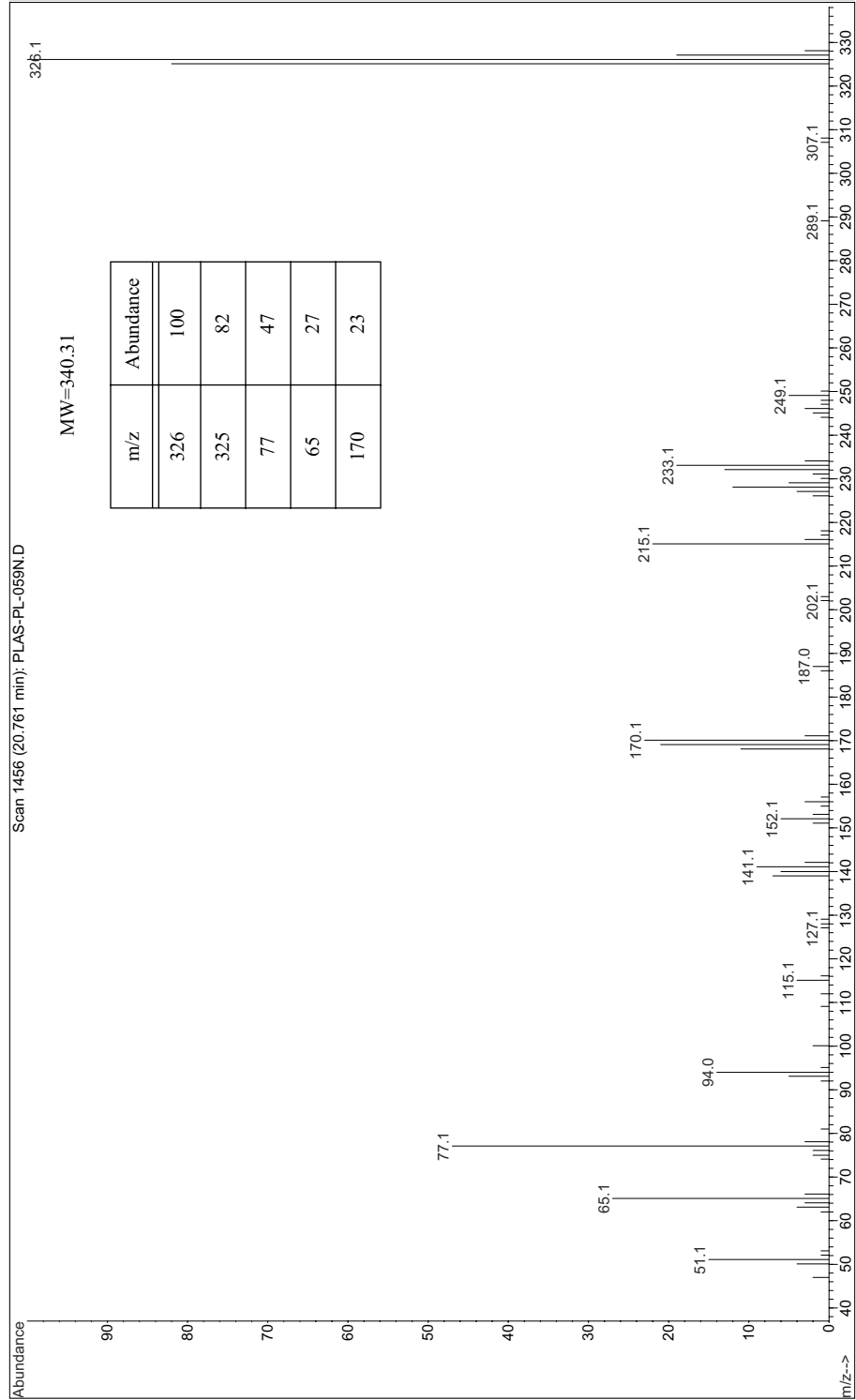
Toxicological Data

LD50 (oral): 6400 mg/kg [Rat].

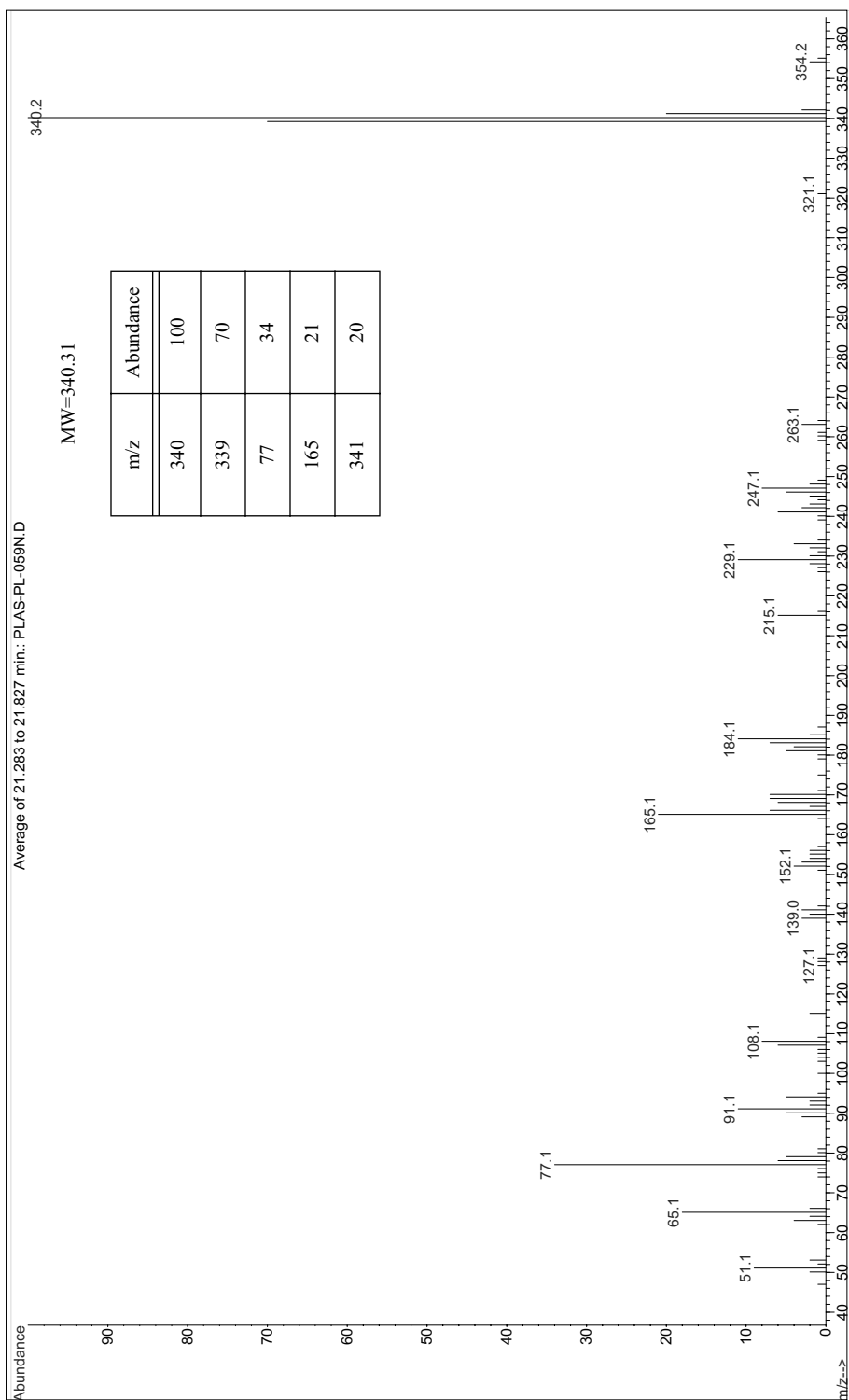
LDLo (dermal): 3160 mg/kg [Rabbit].

LC50 (inhalation) > 0.37 mg/L/1 hour [Sheep].

Mass Spectrum for Cresyl Diphenyl Phosphate - PLAS-PL-059

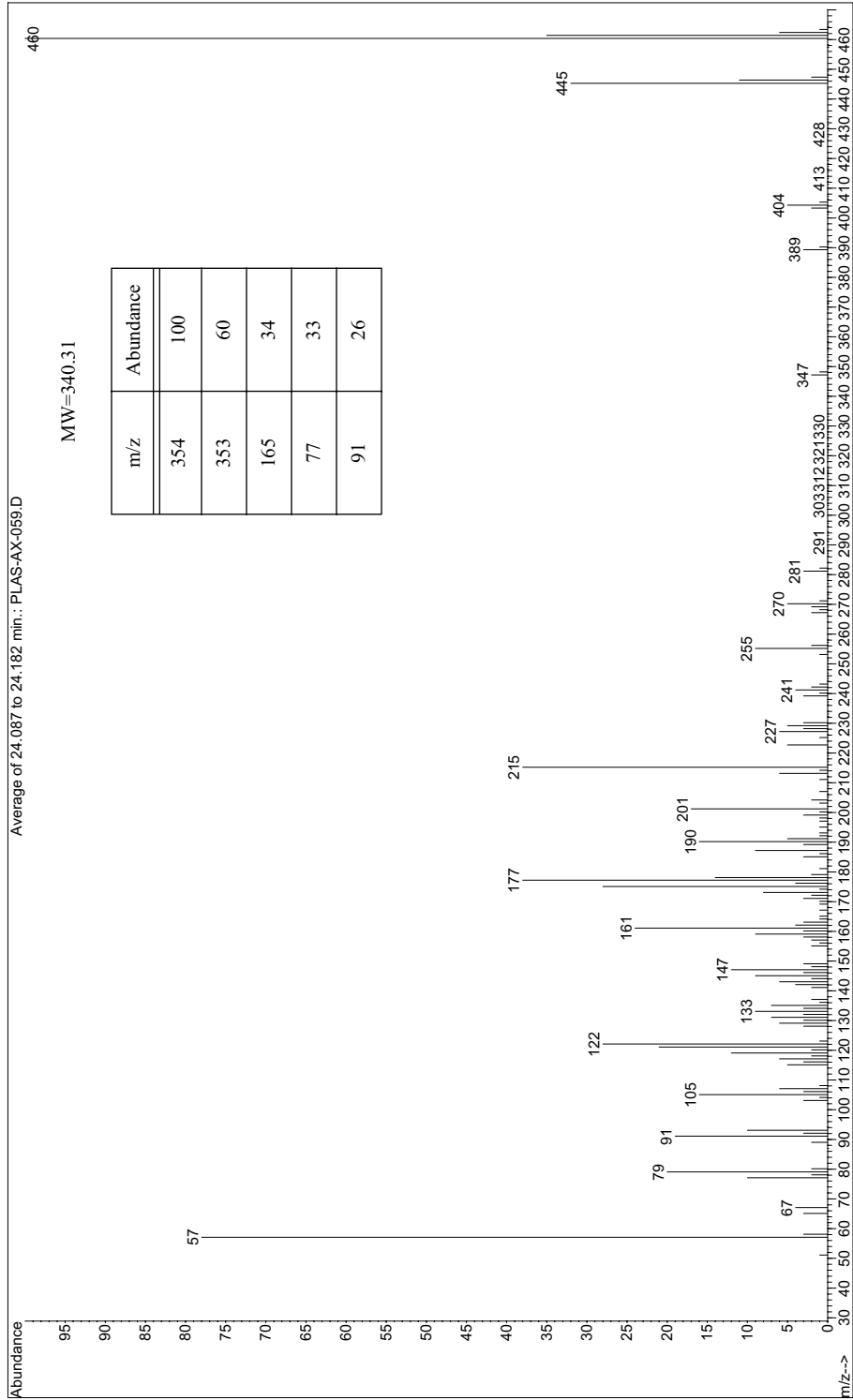


For Chromatogram See Appendix A - PLAS-PL-059 - page 552

Mass Spectrum for Cresyl Diphenyl Phosphate - PLAS-PL-059

For Chromatogram See Appendix A - PLAS-PL-059 - page 552

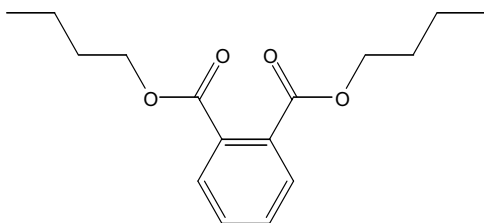
Mass Spectrum for Cresyl Diphenyl Phosphate - PLAS-PL-059



For Chromatogram See Appendix A - PLAS-PL-059 - page 552

Dibutyl phthalate

Houghton Chemical

**CAS Number** 84-74-2**RTECS Number** TI0875000**Abbreviation** DBP**Formula** C₁₆H₂₂O₄**Molecular Weight** 278.34**Chemical Name**

dibutyl phthalate

Synonyms

1,2-benzenedicarboxylic acid, dibutyl ester; n-butyl phthalate

Brand Names & Manufacturers

Morflex® 140

Morflex, Inc.

Polycizer® DBP

Harwick Chemical Corporation

Physical Properties**Appearance** Colorless to yellow, viscous liquid**Melting Point** -35 °C**Boiling Point** 340 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	1	1	1	1	1

Application, Regulatory & Environmental Information

Application Plasticizer used in nitrocellulose lacquers, elastomers, explosives, nail polish, and solid rocket propellants; solvent for perfume oils; perfume fixative; textile lubricating agent; safety glass; insecticides; printing inks; resin solvent; paper coatings; adhesives; and insect repellent for textiles.

Regulatory Information

Regulated by the EPA under the Clean Water Act as a toxic pollutant. EU Directive 2005/84/EC (so called Phthalate Directive) restricts the use of DBP in toys and childcare articles.

Environmental Impact

This substance is toxic to aquatic organisms. The reported log Kow value is 4.77, which indicates a moderate potential to bioaccumulate. The chemical is biodegradable but tends to partition into sediment where it is relatively persistent.

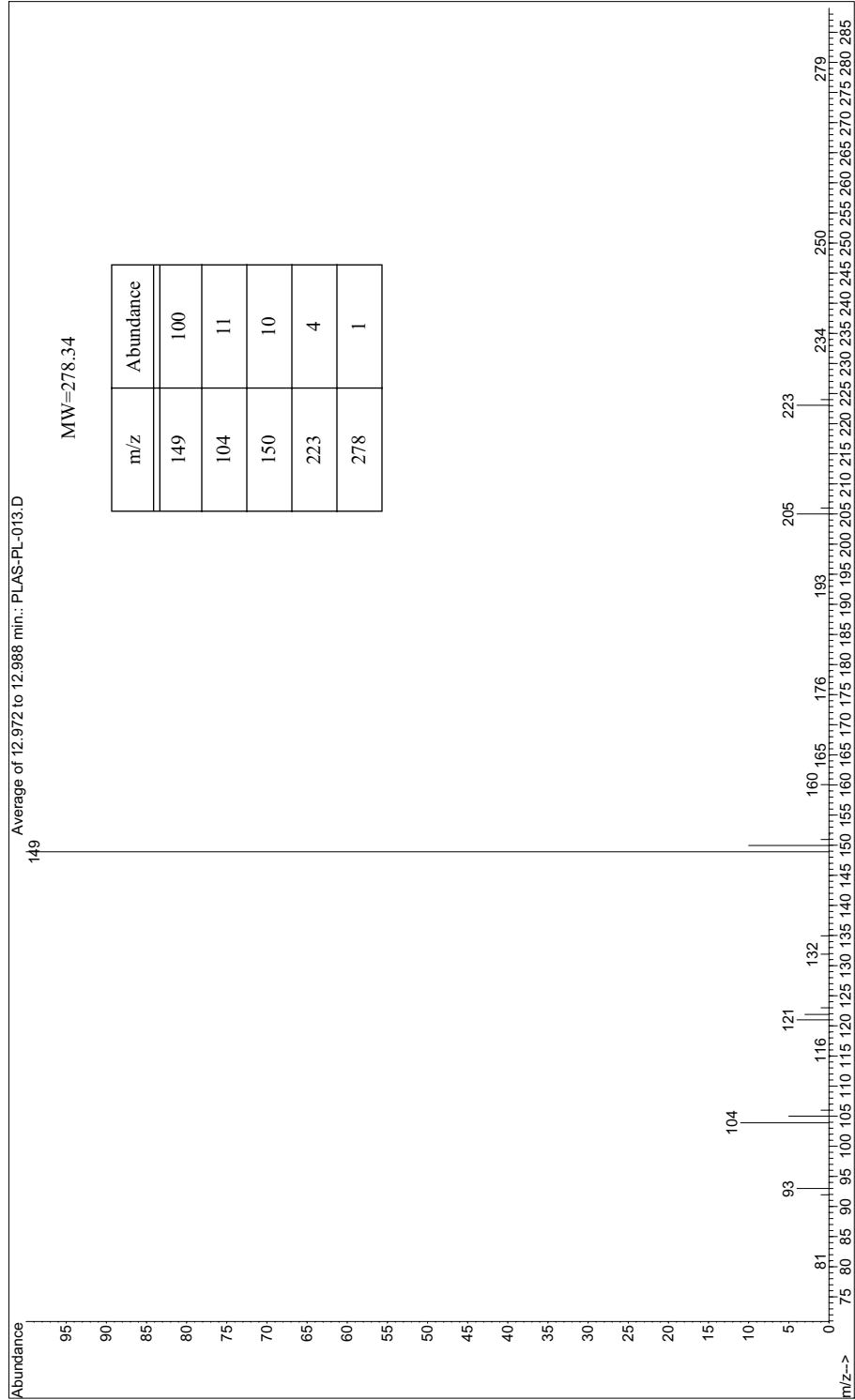
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

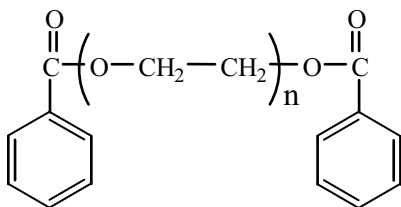
Toxicological Data

Acute oral toxicity (LD50): 7499 mg/kg [Rat]; acute inhalation toxicity (LD50): 4250 mg/m³ [Rat]; acute dermal toxicity (LD50): 6 g/kg [Rat]. Listed on CA Proposition 65 as a chemical known to have developmental toxicity.

Mass Spectrum for Dibutyl phthalate - PLAS-PL-013



For Chromatogram See Appendix A - PLAS-PL-013 - page 553

Dibutyl Sebacate**CAS Number** 109-43-3**RTECS Number** VS1150000**Abbreviation** DBS**Formula** C₁₈H₃₄O₄**Molecular Weight** 314.46**Chemical Name**

Dibutyl decanedioate

Synonyms

N/A

Brand Names & Manufacturers

Kodaflex DBS

Eastman Chemical

Polycizer DBS

Physical Properties**Appearance** Clear liquid**Melting Point** -10 °C**Boiling Point** 344-345 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water 0.004	MeOH S	EtOH S	Acetone U	CH₂Cl₂ U	Hexane U
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Application *Application, Regulatory & Environmental Information*

Used as a plasticizer in production of plastics, namely cellulose acetate butyrate, cellulose acetate propionate, ethyl cellulose, polyvinyl butyral, polyvinyl chloride, polystyrene, and many synthetic rubbers (especially nitrile rubber and neoprene).

Regulatory Information

FDA 21CFR (Indirect and direct food contact) §175.105, §175.5150, §175.300, §175.320, §177.2600 §178.3910.

Environmental Impact

Contains no hazardous air pollutants or ozone depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

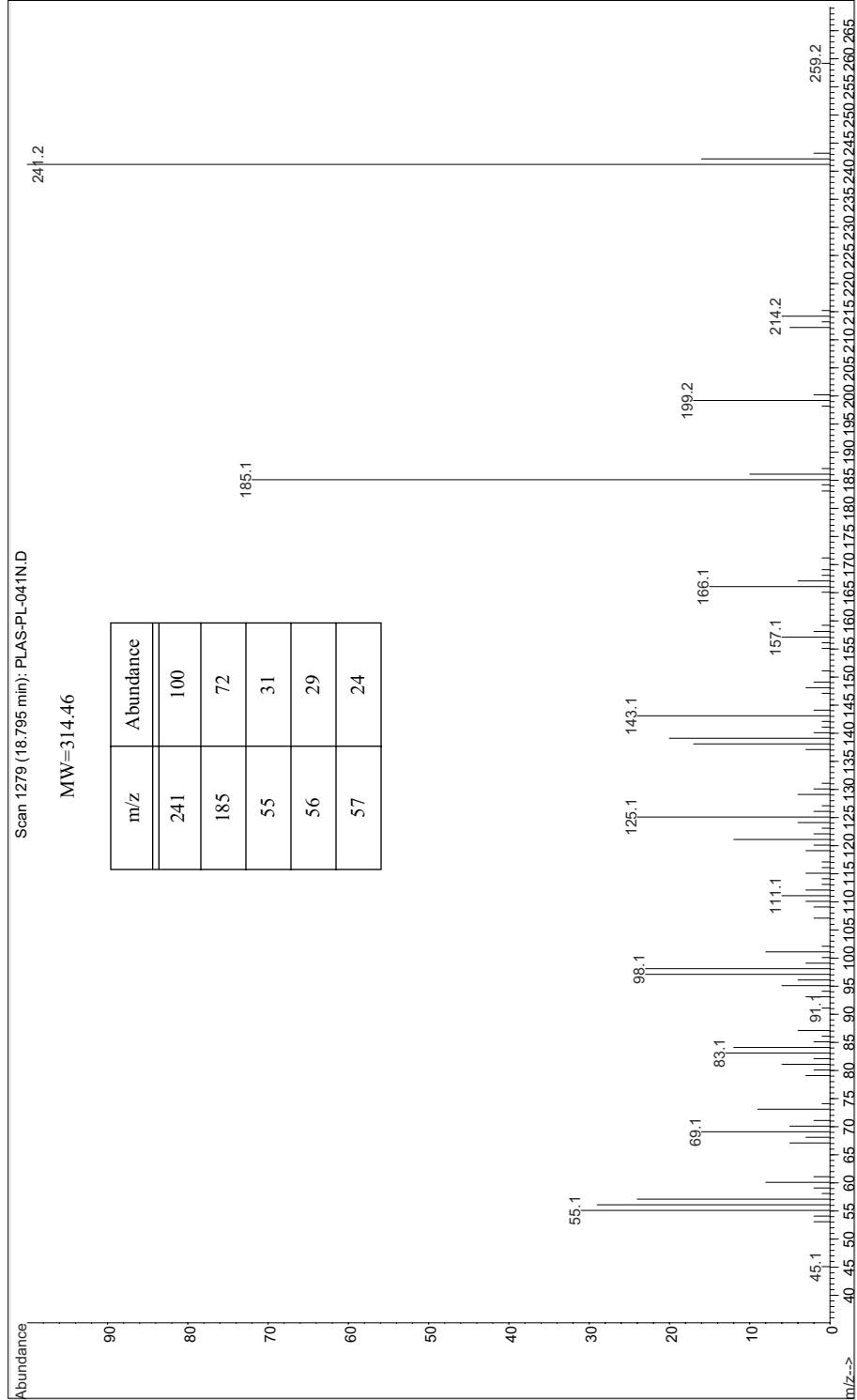
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

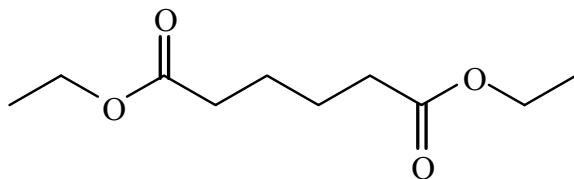
Toxicological Data

Oral LD50: >5000.00 mg/kg [Rat].

Mass Spectrum for Dibutyl Sebacate - PLAS-PL-041



For Chromatogram See Appendix A - PLAS-PL-041 - page 554

Diethyl adipate**CAS Number** 141-28-6**RTECS Number** AV1100000**Abbreviation** Not Identified**Formula** C₁₀H₁₈O₄**Molecular Weight** 202.25**Chemical Name**

hexanedioic acid, diethyl ester

Synonyms

1,6-diethyl hexanedioate; adipic acid, diethyl ester

Brand Names & Manufacturers

Sold as bulk chemical

Varied

Physical Properties**Appearance** Colorless liquid**Melting Point** -19.8 °C**Boiling Point** 245 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane 40-80
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Application, Regulatory & Environmental Information

Application Plasticizer for vinyl resins and solvent carriers or coupling agents for polyurethane and photographic films. Typically used in combination with phthalates.

Regulatory Information

Not approved by the FDA for food contact applications.

Environmental Impact

Listed by the EPA as a non-hazardous chemical. Diethyl adipate is readily biodegradable and has a low potential to bioaccumulate based on a measured log Kow value of 1.79.

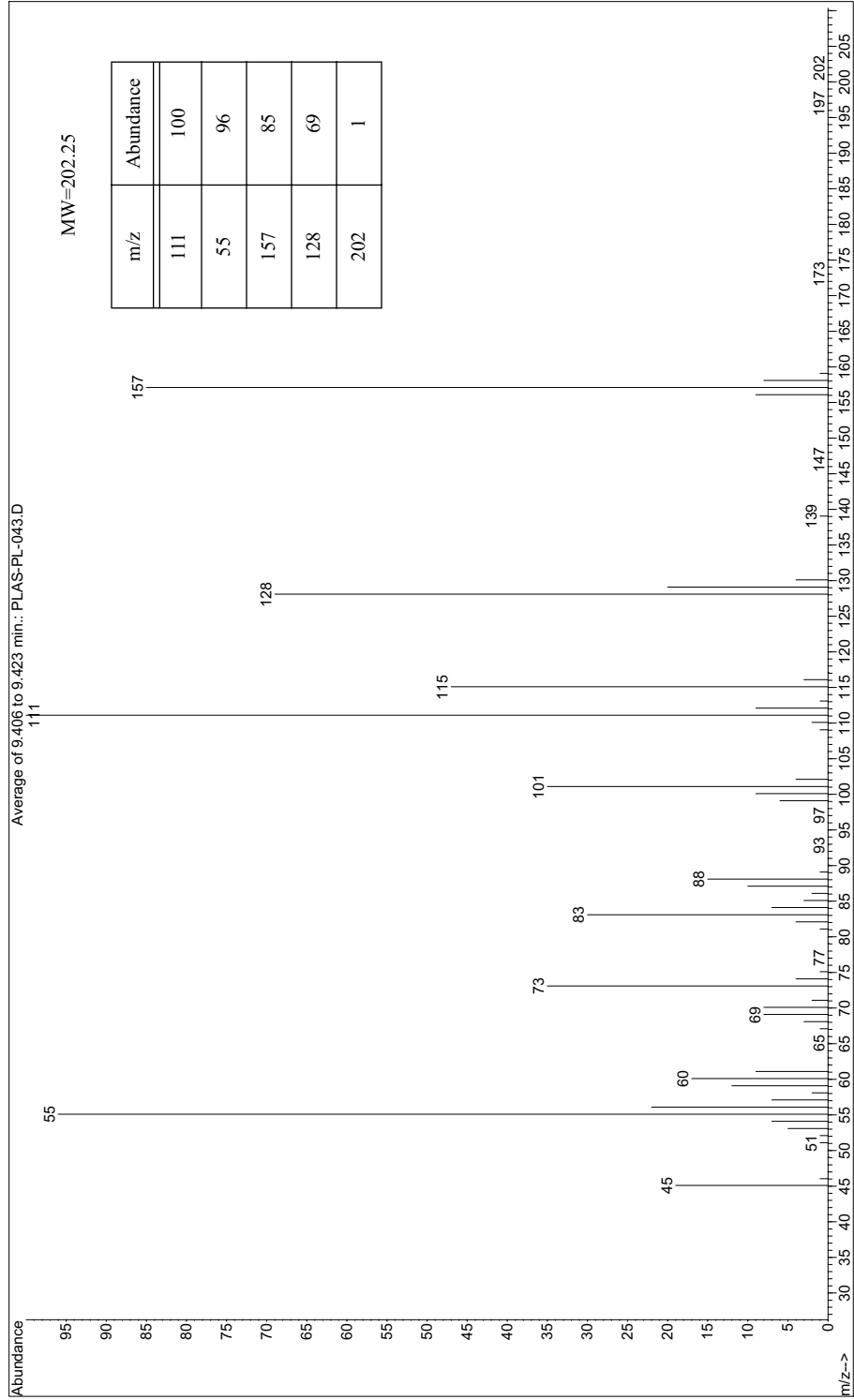
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

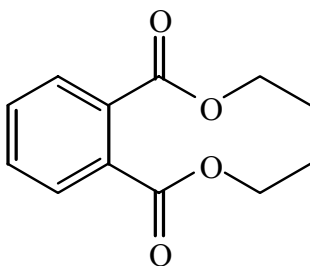
Toxicological Data

Oral LD50: 8100 mg/kg [Mouse], intraperitoneal LD50: 2190 mg/kg [Mouse]. Chronic Exposure — Teratogen: Dose: 837 mg/kg [Rat], intraperitoneal exposure time: (5–15 d PREG) resulted in developmental abnormalities and fetal death. Chronic Exposure — Mutagen: Dose: 1100 mg/kg [Mouse], intraperitoneal dose: 1100 mg/kg. Mutation test: Dominant lethal test.

Mass Spectrum for Diethyl adipate - PLAS-PL-043



For Chromatogram See Appendix A - PLAS-PL-043 - page 555

Diethyl phthalate**CAS Number** 84-66-2**RTECS Number** TI1050000**Abbreviation** DEP**Formula** C₁₂H₁₄O₄**Molecular Weight** 222.24**Chemical Name**

1,2-benzenedicarboxylic acid, diethyl ester

Synonyms

diethyl phthalate; diethyl 1,2-benzenedicarboxylate; o-bis(ethoxycarbonyl)benzene; phthalic acid, diethyl ester

Brand Names & Manufacturers

Sold as bulk chemical

Various

Physical Properties**Appearance** Clear oily liquid**Melting Point** -40.5 °C**Boiling Point** 295 °C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂ U	Hexane
	<0.1	40-80	40-80	40-80		40-80

Application, Regulatory & Environmental Information**Application**

DEP is used as a plasticizer to make plastics more flexible. Commonly found in products such as toothbrushes, automobile parts, tools, toys, and food packaging. Also used as a plasticizer in solid rocket propellants and cellulose ester plastics such as photographic films and sheets, blister packaging, and tape applications.

Regulatory Information

SARA 313 reportable chemical. Classified as environmentally hazardous for shipping purposes. EPA regulated under the Clean Water Act.

Environmental Impact

Diethyl phthalate is designated a toxic pollutant under the Clean Water Act. This substance may be hazardous to the environment; special attention should be given to fish.

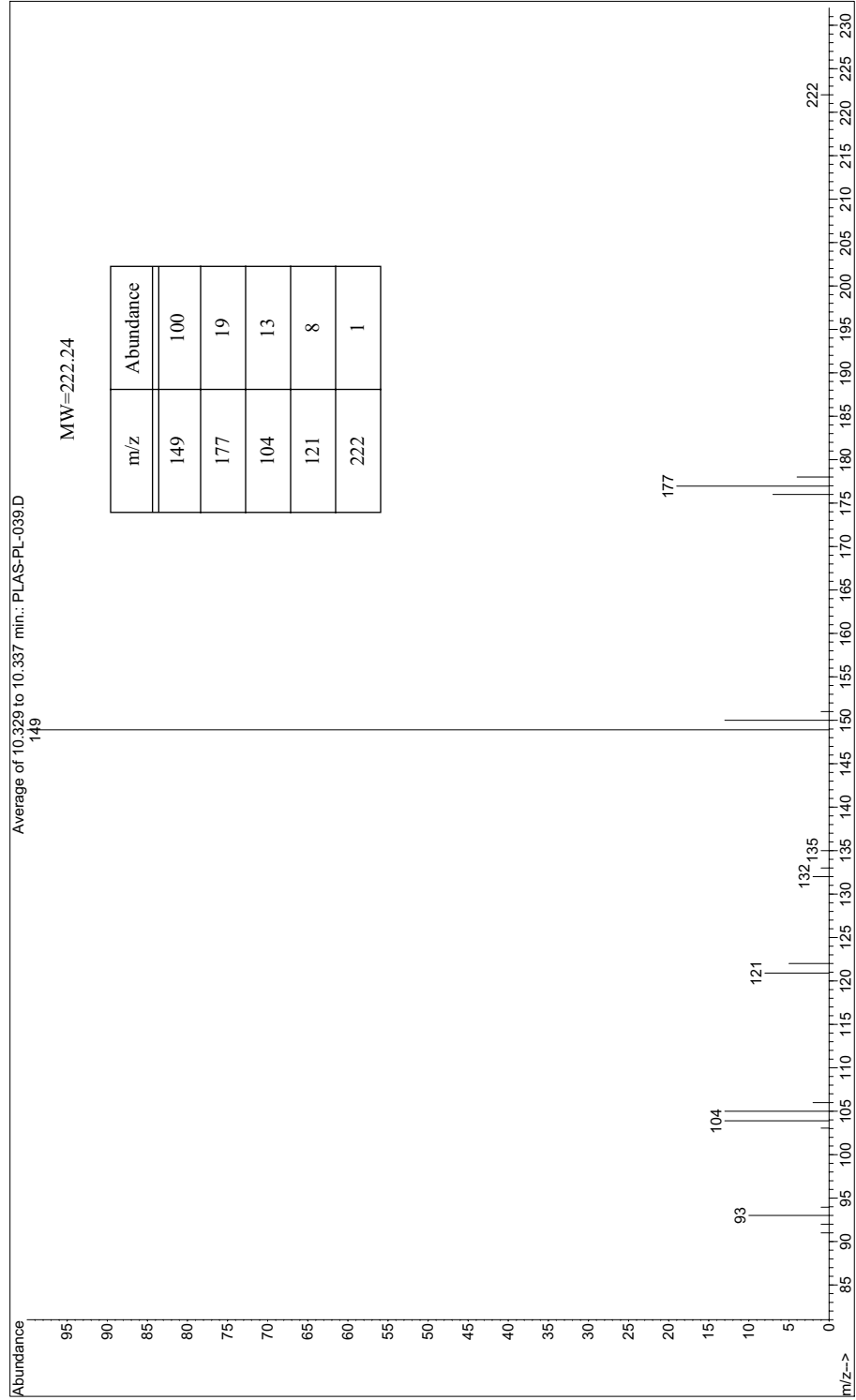
Point of Release

Because diethyl phthalate is not a part of the chain of chemicals, or polymers, which makes up the plastics, it can be released fairly easily from products in which it is used. Exposure may occur when you use plastics that contain it, and when you eat food from plastic containers made with it. This substance has been found in at least 248 of the 1430 National Priorities List sites identified by the Environmental Protection Agency (EPA).

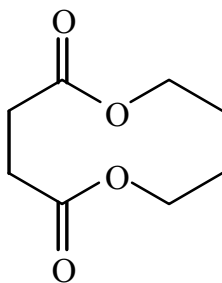
Toxicological Data

Oral (LD50): 9000 mg/kg [Rat], 1000 mg/kg [Rabbit]; Inhalation (LC50): > 4640 mg/m³ [Rat]; skin (LD50) > 20 mg/kg [Guinea pig].

Mass Spectrum for Diethyl phthalate - PLAS-PL-039



For Chromatogram See Appendix A - PLAS-PL-039 - page 556

Diethyl succinate**CAS Number** 123-25-1**RTECS Number** WM7400000**Abbreviation** Not Identified**Formula** C₈H₁₄O₄**Molecular Weight** 174.19**Chemical Name**

butanedioic acid, diethyl ester

Synonyms

ethyl succinate; diethyl butanedioate; succinic acid; diethyl ester

Brand Names & Manufacturers

Sold as bulk chemical

Varied

Physical Properties**Appearance** Colorless liquid**Melting Point** -21.0 °C**Boiling Point** 217.7 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.2	40-80	40-80	U	U	U

Application, Regulatory & Environmental Information**Application**

Plasticizer for PVC resins.

Regulatory Information

Diethyl succinate has FDA approval for use as a food additive. Also approved for use in a wide variety of food contact applications.

Environmental Impact

Possibly hazardous short-term degradation products are not likely. However, long-term degradation products may arise. The product itself and its products of degradation are not toxic to the environment.

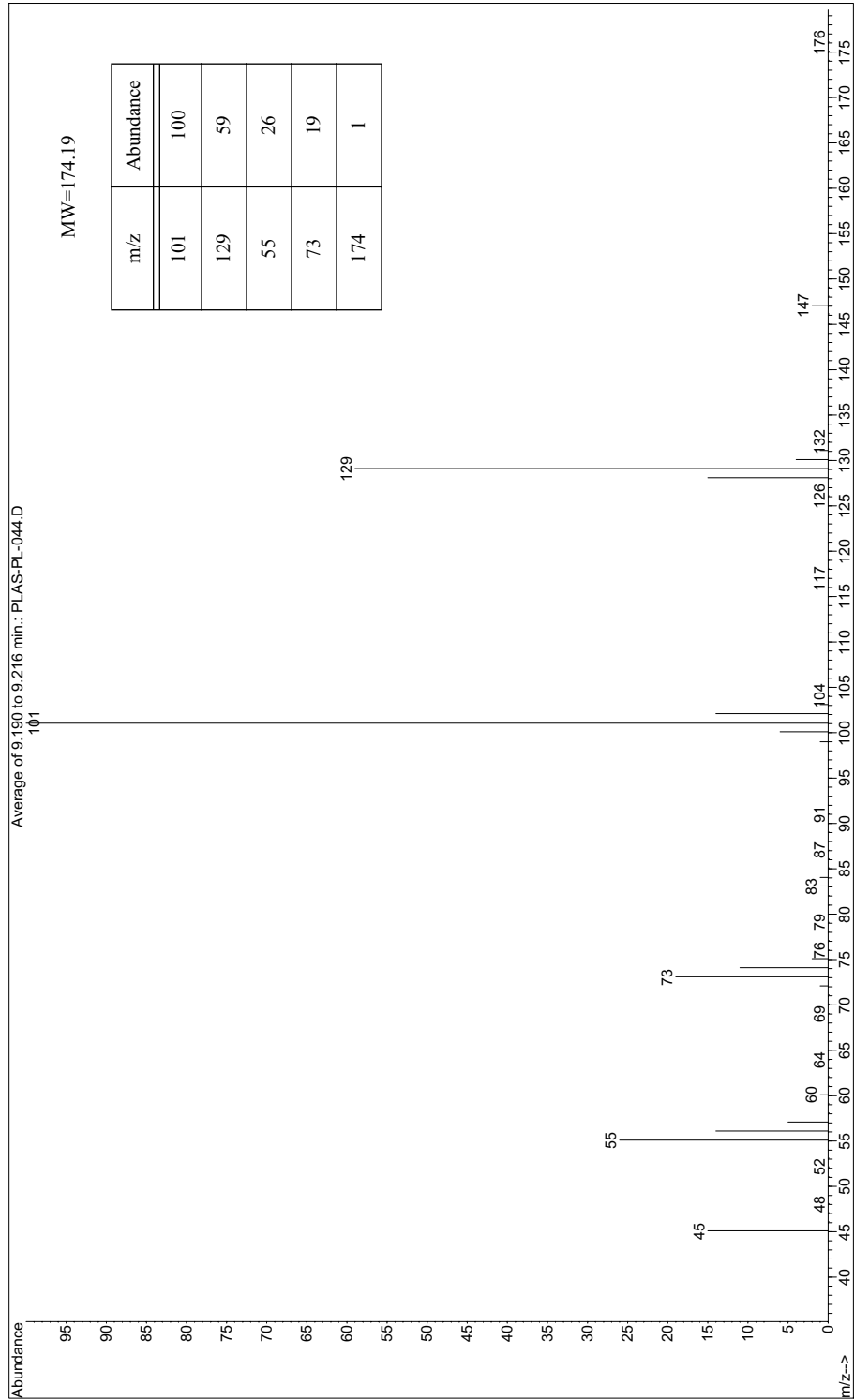
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

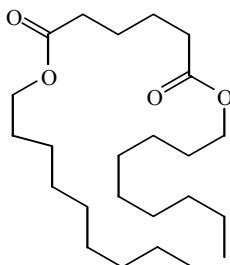
Toxicological Data

Oral (LD50): 8530 mg/kg [Rat]. Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectrum for Diethyl succinate - PLAS-PL-044



For Chromatogram See Appendix A - PLAS-PL-044 - page 557

Diisononyl adipate**CAS Number** 33703-08-1**RTECS Number** N/A**Abbreviation** DINA**Formula** C₂₄H₄₆O₄**Molecular Weight** 398.63**Chemical Name**

hexanedioic acid, diisononyl ester

Synonyms

bis(isononyl)adipate; diisononyl hexanedioate; adipic acid; diisononyl ester

Brand Names & Manufacturers

Jayflex® DINA

ExxonMobil

Plastomoll® DNA

BASF

Santicizer® DINA

Solutia Inc.

Physical Properties**Appearance** Clear liquid**Melting Point** -65 °C**Boiling Point** 235 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application**

Diisononyl adipate is a highly efficient plasticizer that imparts low temperature flexibility and impact resistance to the base resin. Widely used in shrinkwrap, electrical wire jackets, and films. Also used in sausage casings.

Regulatory Information

Approved by the FDA for use as a food additive and/or food contact material.

Environmental Impact

Adipates are sensitive to hydrolysis, recovering the acid and alcohols particularly under alkaline conditions. This contributes to their ability to degrade easily in the environment. Log Kow value of 9.24 indicates a potential to bioaccumulate. They are reported to have an acute toxicity to aquatic wildlife.

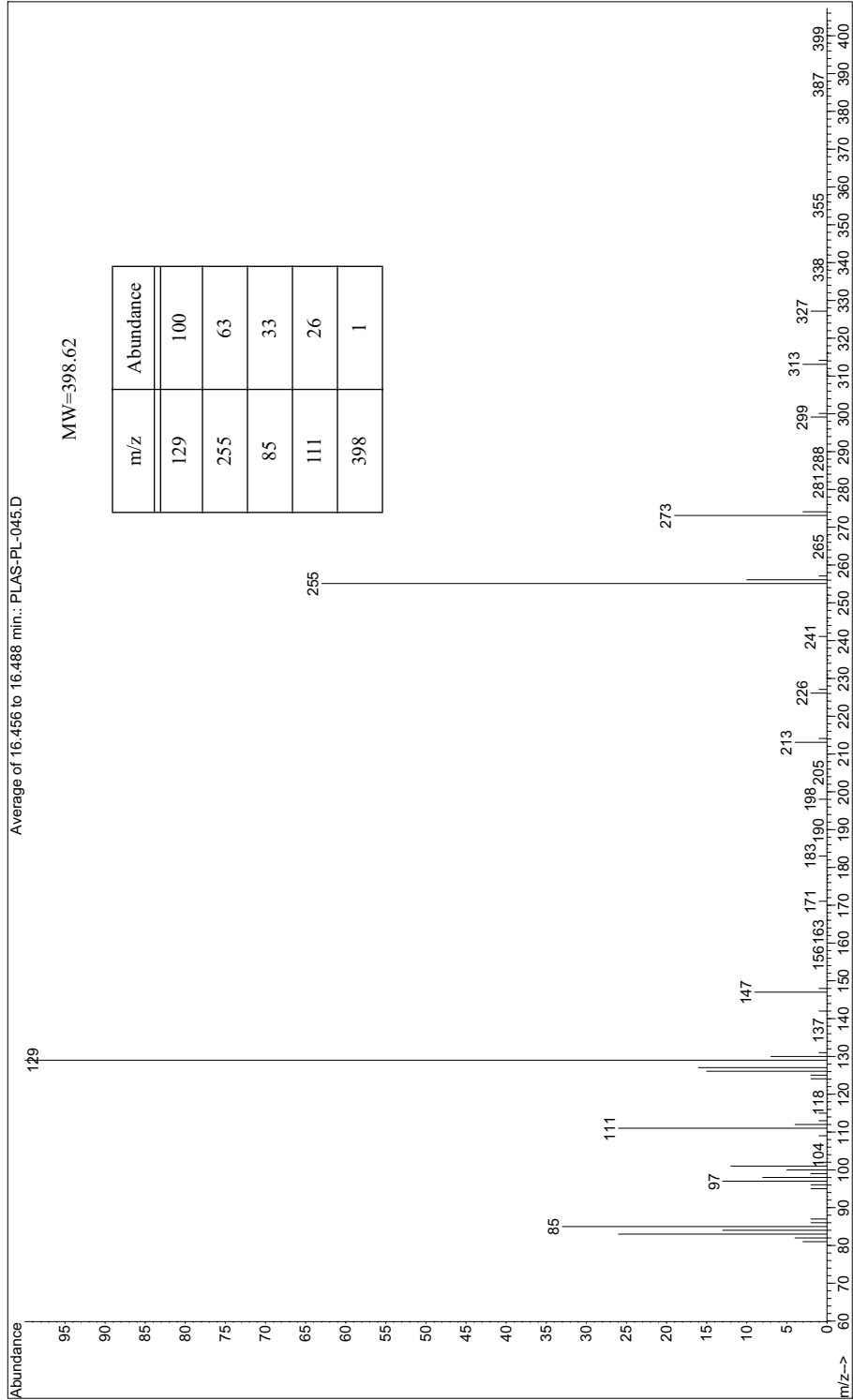
Point of Release

High-level contamination of DINA has been found in fish-paste products and other packaged foods, presumably because of migration from plasticized wrapping film used for food packaging.

Toxicological Data

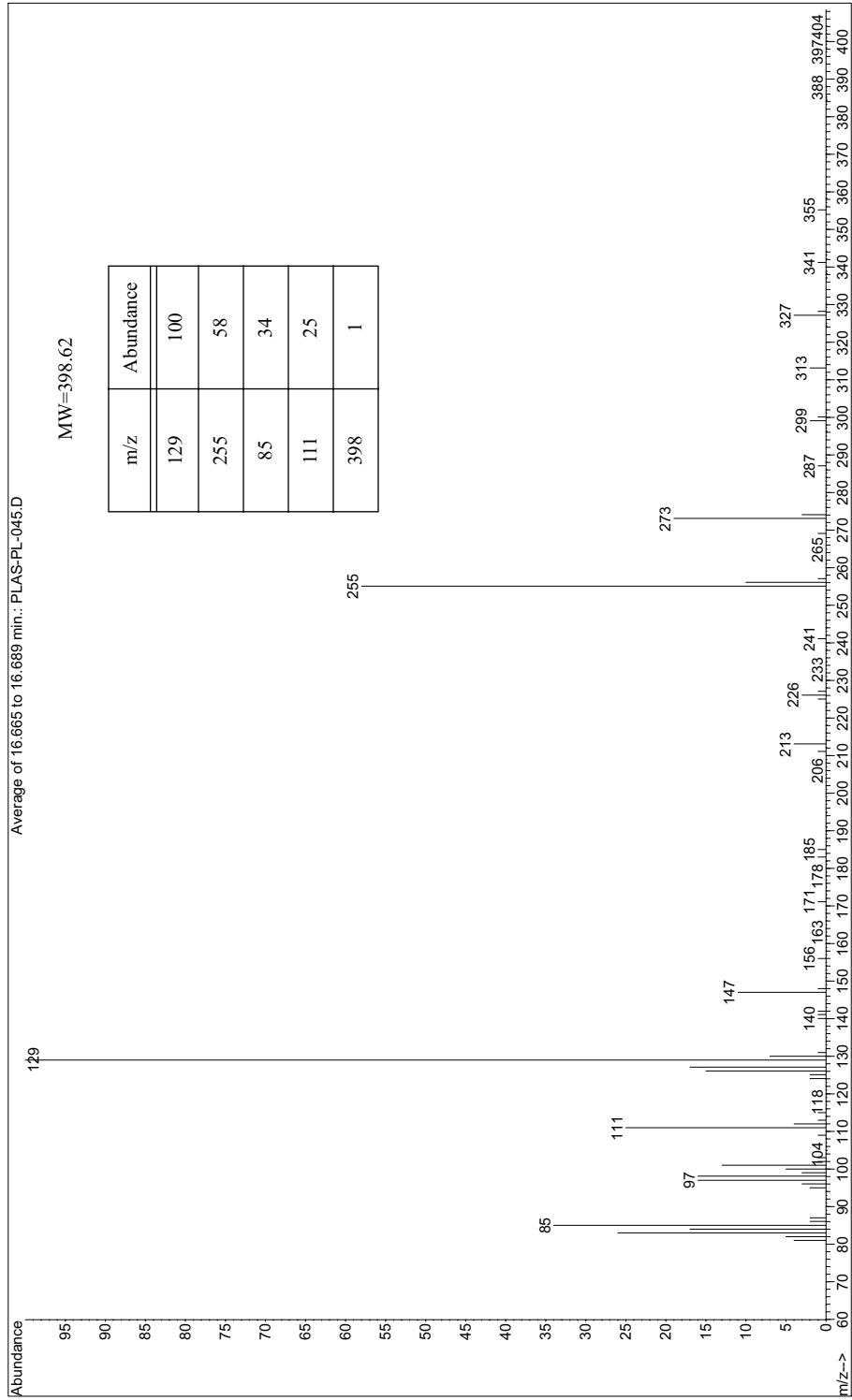
Concern over the mutagenic and carcinogenic potential of these materials was stimulated by the finding that one member of this class, di-(2-ethylhexyl) adipate (DEHA), induced liver tumors in female mice in a chronic feeding study. Accordingly, the genotoxic potential of DINA was evaluated in a battery of in vitro tests and did not exhibit any evidence of mutagenic or transforming potential in any of the assays utilized.

Mass Spectrum for Diisononyl adipate - PLAS-PL-045



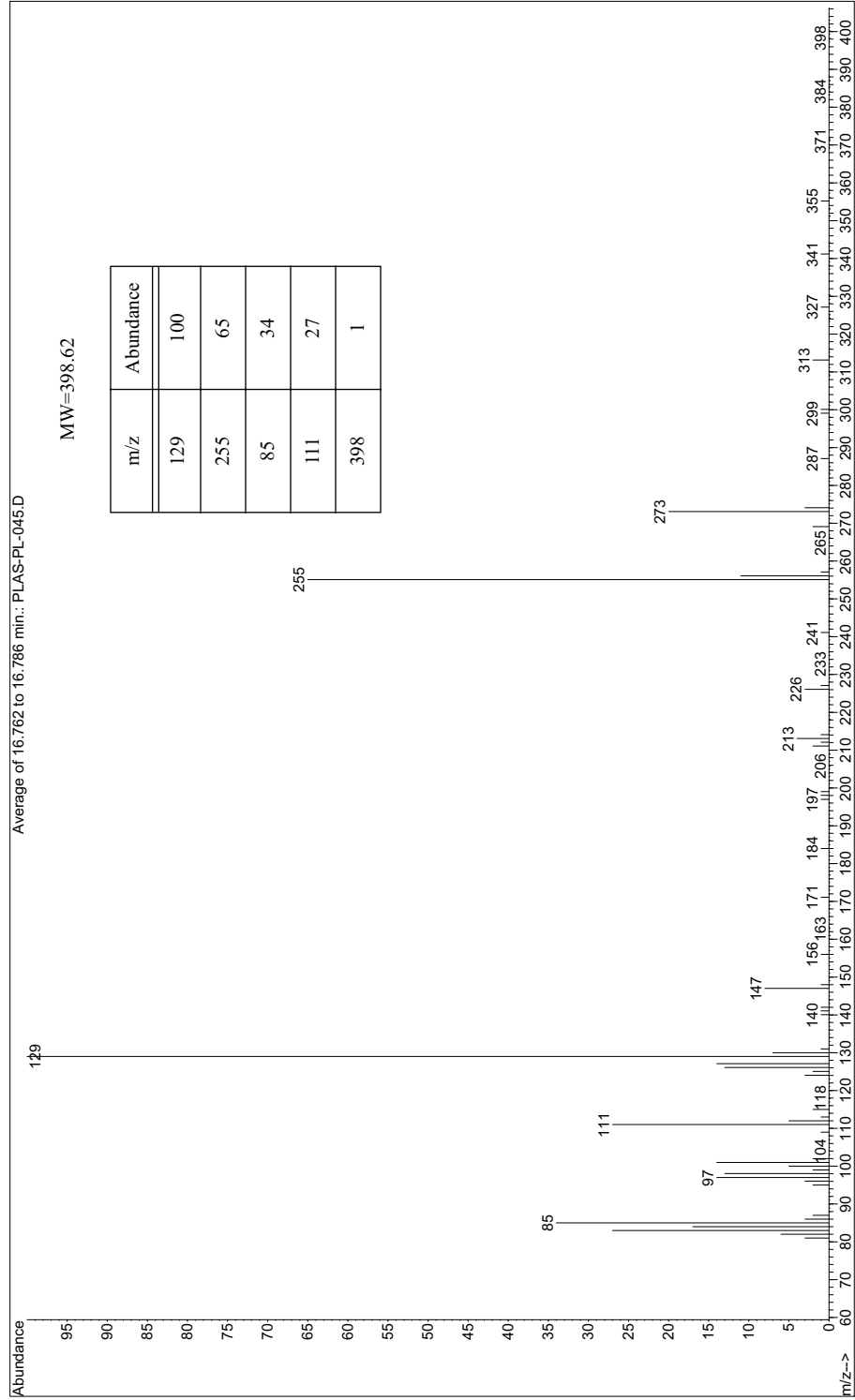
For Chromatogram See Appendix A - PLAS-PL-045 - page 558

Mass Spectrum for Diisononyl adipate - PLAS-PL-045

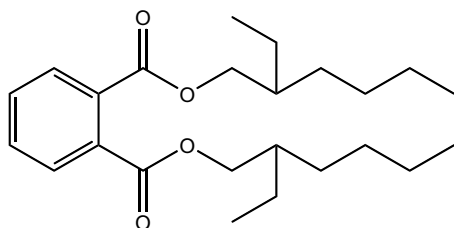


For Chromatogram See Appendix A - PLAS-PL-045 - page 558

Mass Spectrum for Diisononyl adipate - PLAS-PL-045



For Chromatogram See Appendix A - PLAS-PL-045 - page 558

Diisooctyl phthalate**CAS Number** 27554-26-3**RTECS Number** TI1300000**Abbreviation** DIOP**Formula** C₂₄H₃₈O₄**Molecular Weight** 390.56**Chemical Name**

bis(6-methylheptyl) benzene-1,2-dicarboxylate

Synonyms

diisocapryl phthalate; diisooctyl 1,2-benzenedicarboxylate

Brand Names & Manufacturers

Corflex 880

Jayflex DIOP

Exxon Mobil

Physical Properties**Appearance** Clear liquid**Melting Point** -56 °C**Boiling Point** 208-209 °C**Stability** Stable under normal conditions of use.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.01	U	U	S	S	S

Application, Regulatory & Environmental Information**Application**

Used primarily to make soft and flexible polyvinyl chloride (PVC) for the applications in the industry of automotive, building and construction material, cable, flooring, medical devices, and toys.

Regulatory Information

FDA approved for use in adhesives as a component of articles intended for use in packaging, transporting, or holding food in accordance with the conditions prescribed by 21 CFR §175.105, and as an ingredient in the manufacture of resinous and polymeric coatings of food-contact surface of articles intended for use in producing, manufacturing, packing, transporting, or holding food in accordance with 21 CFR §175.300.

Environmental Impact

Diisooctyl phthalate is expected to adsorb to suspended solids and sediment. A measured BCF of 207 in mosquito fish suggests a high threshold for environmental concern and a moderate potential to bioaccumulate.

Point of Release

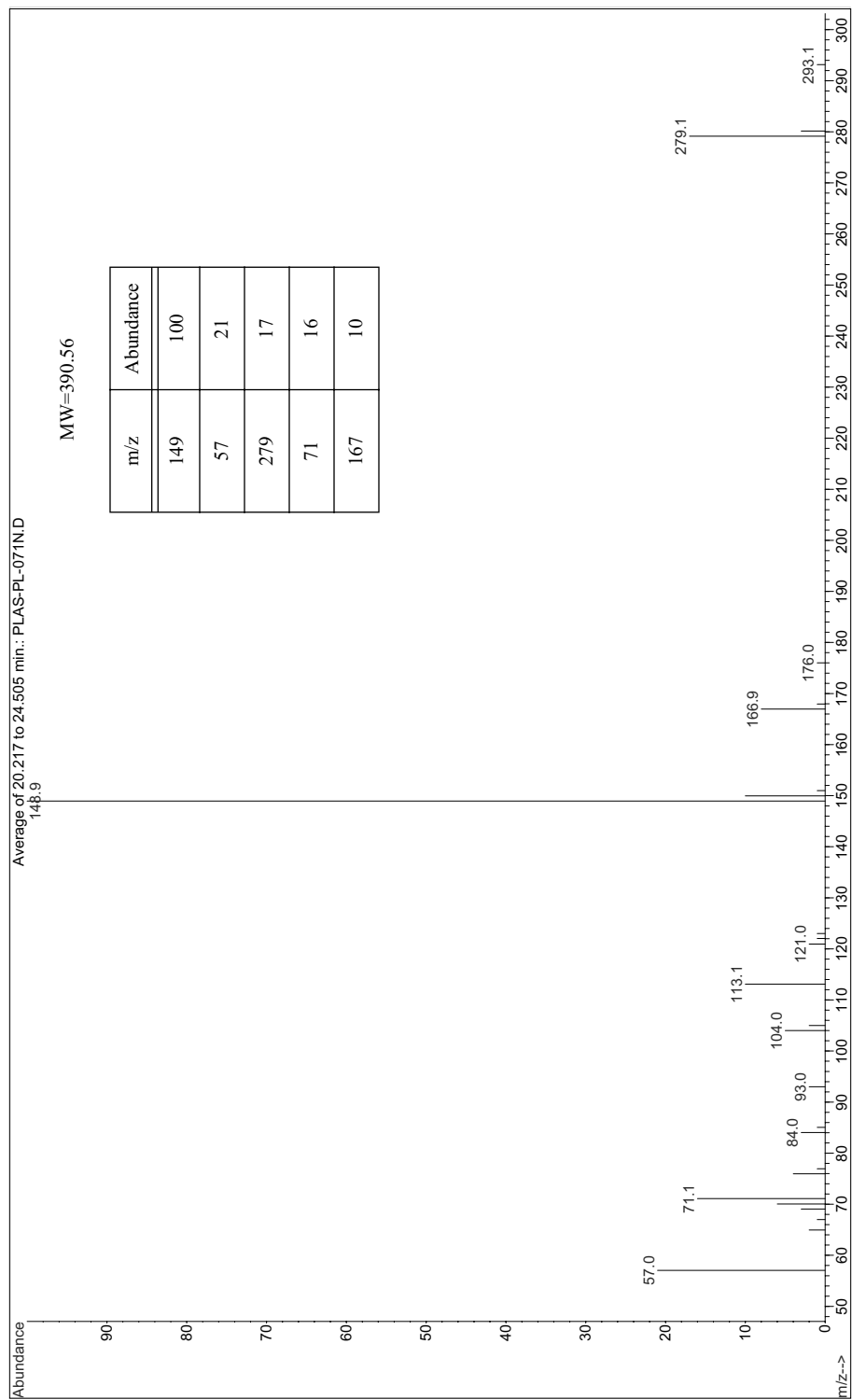
Occupational exposure to diisooctyl phthalate may occur through inhalation and dermal contact with this compound at workplaces where it is produced or used. Use data indicate that the general population may be exposed to diisooctyl phthalate via dermal contact with consumer products containing this compound.

Toxicological Data

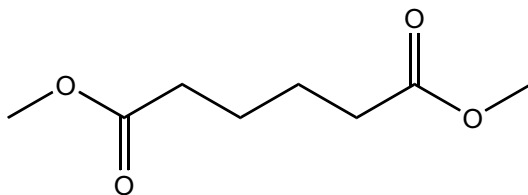
Oral: >22000 mg/kg bw/d [Rat]; oral >26000 mg/kg bw [Mouse]; dermal: >3160 mg/kg bw [Rabbit].

DIOP is generally considered to be of low toxicity via the oral and dermal routes. Mucous membrane and eye irritation may occur. Central nervous system depression may occur. Dermal irritation is seldom seen. Skin sensitization does not occur in humans.

Mass Spectrum for Diisooctyl phthalate - PLAS-PL-071



For Chromatogram See Appendix A - PLAS-PL-071 - page 559

Dimethyl adipate**CAS Number** 627-93-0**RTECS Number** AV1645000**Abbreviation** DMA**Formula** C₈H₁₄O₄**Molecular Weight** 174.19**Chemical Name**

dimethyl hexanedioate

Synonyms

hexanedioic acid dimethyl ester; adipic acid; dimethyl ester

Brand Names & Manufacturers

DBE 6

DuPont

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** 8 °C**Boiling Point** 109-110 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.6	S	S	U	U	U

Application, Regulatory & Environmental Information

Application Used as low-temperature-resistant and low-viscosity plasticizer for PVC and its copolymers and cellulose esters (e.g., cellulose acetate butyrates and cellulose propionates). They are also used as solvent carriers or coupling agents for polyurethane.

Regulatory Information

Not hazardous according to Directive 67/548/EEC.

Environmental Impact

Not expected to bioaccumulate or have significant negative impact to aquatic organisms.

Point of Release

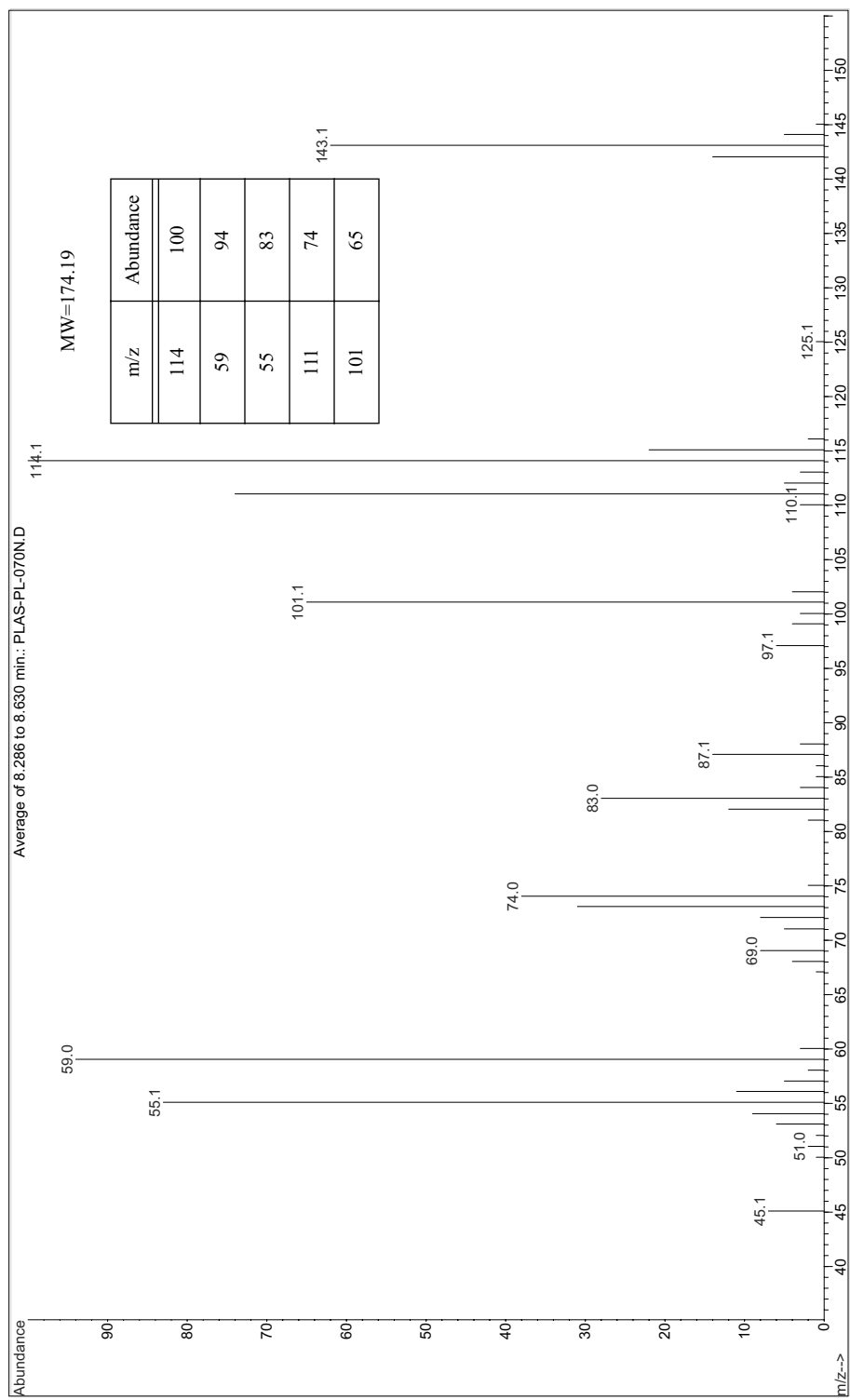
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

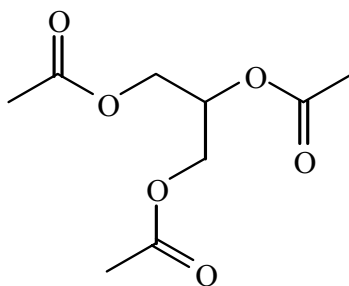
TDLo intraperitoneal 362 mg/kg female 5 to 15 days of pregnancy [Rat].

Effects on fertility — Post-implantation mortality.

Mass Spectrum for Dimethyl adipate - PLAS-PL-070



For Chromatogram See Appendix A - PLAS-PL-070 - page 560

Dimethyl Sebacate**CAS Number** 106-79-6**RTECS Number** HD8370000**Abbreviation** DMS**Formula** C₁₂H₂₂O₄**Molecular Weight** 230.30**Chemical Name**

dimethyl decanedioate

Synonyms

sebacic acid dimethyl ester; decanedioic acid; dimethyl ester

Brand Names & Manufacturers

Sold as bulk chemical

Various

Physical Properties**Appearance** colorless liquid**Melting Point** 23 °C**Boiling Point** 288 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
0.3	S	S	S	S	U	U

Application, Regulatory & Environmental Information**Application**

Plasticizer, softening agent, and solvent for cellulose resin, polyethylene resin, and synthetic rubber.

Regulatory Information

FDA 21CFR §177.1630 (Indirect additive used in food contact substances).

Environmental Impact

Contains no hazardous air pollutants or ozone depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

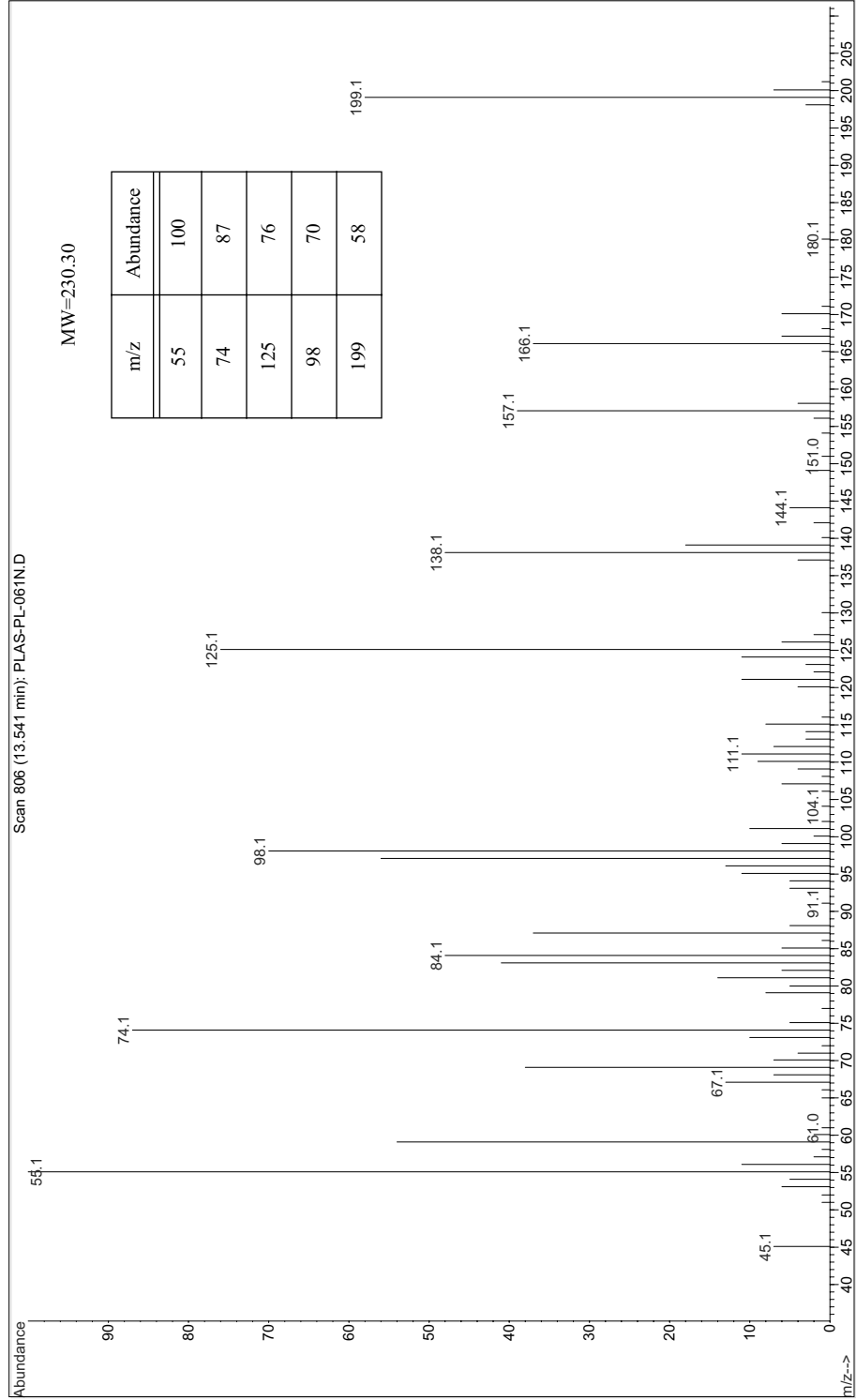
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

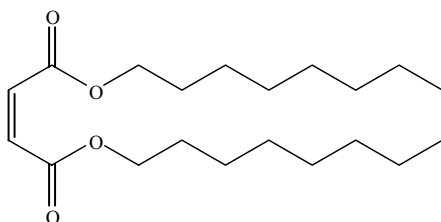
Toxicological Data

DMS does not meet the criteria for high hazard to human health based on classifications by national or international agencies for carcinogenicity, genotoxicity, developmental toxicity, or reproductive toxicity.

Mass Spectrum for Dimethyl Sebacate - PLAS-PL-061



For Chromatogram See Appendix A - PLAS-PL-061 - page 561

Diocetyl maleate**CAS Number** 2915-53-9**RTECS Number** N/A**Abbreviation** DOM**Formula** C₂₀H₃₆O₄**Molecular Weight** 340.50**Chemical Name**

(2Z)-2-butenedioic acid

Synonyms

maleic acid, dioctyl ester

Brand Names & Manufacturers

Sold as bulk chemical

Various

Physical Properties**Appearance** Liquid**Melting Point** -40 °C**Boiling Point** 209 °C**Stability**

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	U	U	U

Application *Application, Regulatory & Environmental Information*

Used as a plasticizer for vinyl resins and for applications involving co-polymerization with polyvinyl chloride and vinyl acetates in emulsion paints and adhesives. Provides elasticity and flexibility.

Regulatory Information

Diocetyl maleate is FDA approved under 21CFR175.105 — Indirect Food Additives — Adhesives.

Environmental Impact

Readily biodegradable and has a low potential to bioaccumulate. Not expected to be toxic to the aquatic environment.

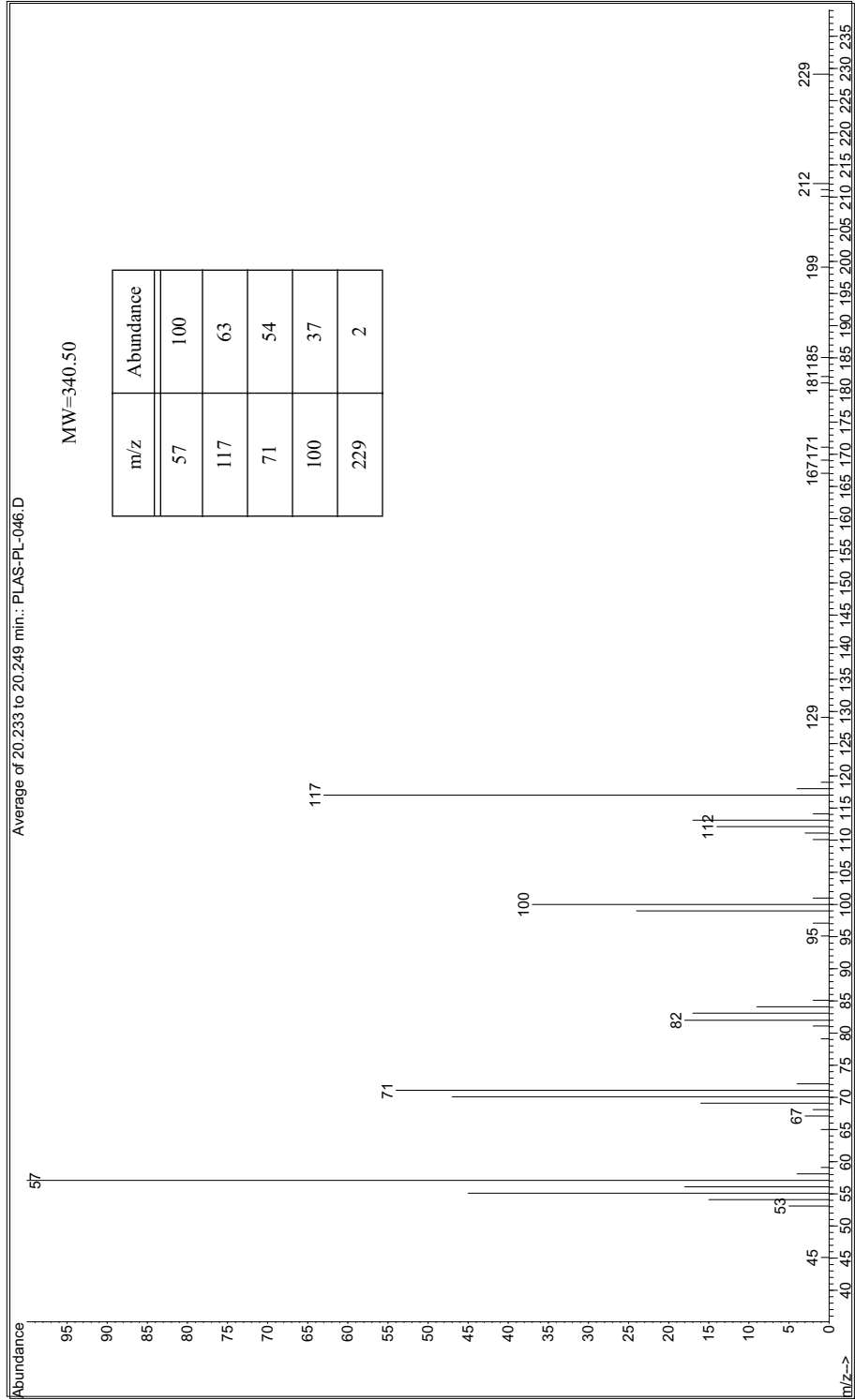
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): 2 to 5 g/kg [Rat]; slightly toxic to animals. Dermal (LD50): 2.6 g/kg [Rabbits]; moderately to severely irritating to rabbit skin. Practically non-toxic to animals. Not a skin sensitizer. Inhalation (LC50): > 0.89 but < 5.3 mg/l [Rat] 4 hour; slightly toxic to animals.

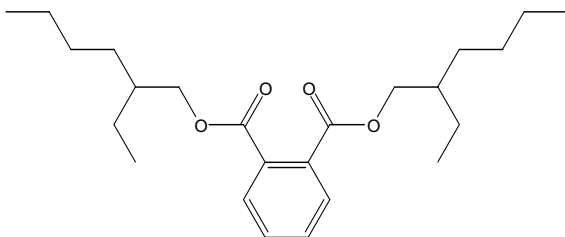
Mass Spectrum for Diocetyl maleate - PLAS-PL-046



For Chromatogram See Appendix A - PLAS-PL-046 - page 562

Diethyl phthalate (DOP)

Houghton Chemical

**CAS Number** 117-81-7**RTECS Number** TI0350000**Abbreviation** DOP**Formula** C₂₄H₃₈O₄**Molecular Weight** 390.56**Chemical Name**

dioctyl phthalate

Synonyms

DOP; bis(2-ethylhexyl)phthalate; di-2-ethylhexyl phthalate

Brand Names & Manufacturers

Plasthall® DOP

C. P. Hall Company

Polycizer® DOP

Harwick Chemical Corporation

Physical Properties**Appearance** Colorless, viscous liquid**Melting Point** -50 °C**Boiling Point** 385 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	40-80	40-80	40-80	1

Application, Regulatory & Environmental Information**Application**

Plasticizer for resins and elastomers which are used to manufacture many products, including teething rings, pacifiers, soft squeeze toys, balls, vinyl upholstery, tablecloths, shower curtains, raincoats, adhesives, polymeric coatings, components of paper and paperboard, defoaming agents, enclosures for food containers, and vinyl gloves used for medical examinations and surgery.

Regulatory Information

EPA regulates DOP under the Clean Water Act (CWA), Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), Resource Conservation and Recovery Act (RCRA), Superfund Amendments and Reauthorization Act (SARA), and Toxic Substances Control Act (TSCA). Listed on CA Prop 65 as a known carcinogen.

Environmental Impact

This material is considered to be moderately toxic to aquatic organisms and will bioaccumulate, especially in fish. When released to soil, it attaches strongly to the soil and does not migrate away from where it was released. When released to water, it dissolves very slowly into underground water or surface waters. It takes many years for DOP in buried or discarded materials to disappear from the environment.

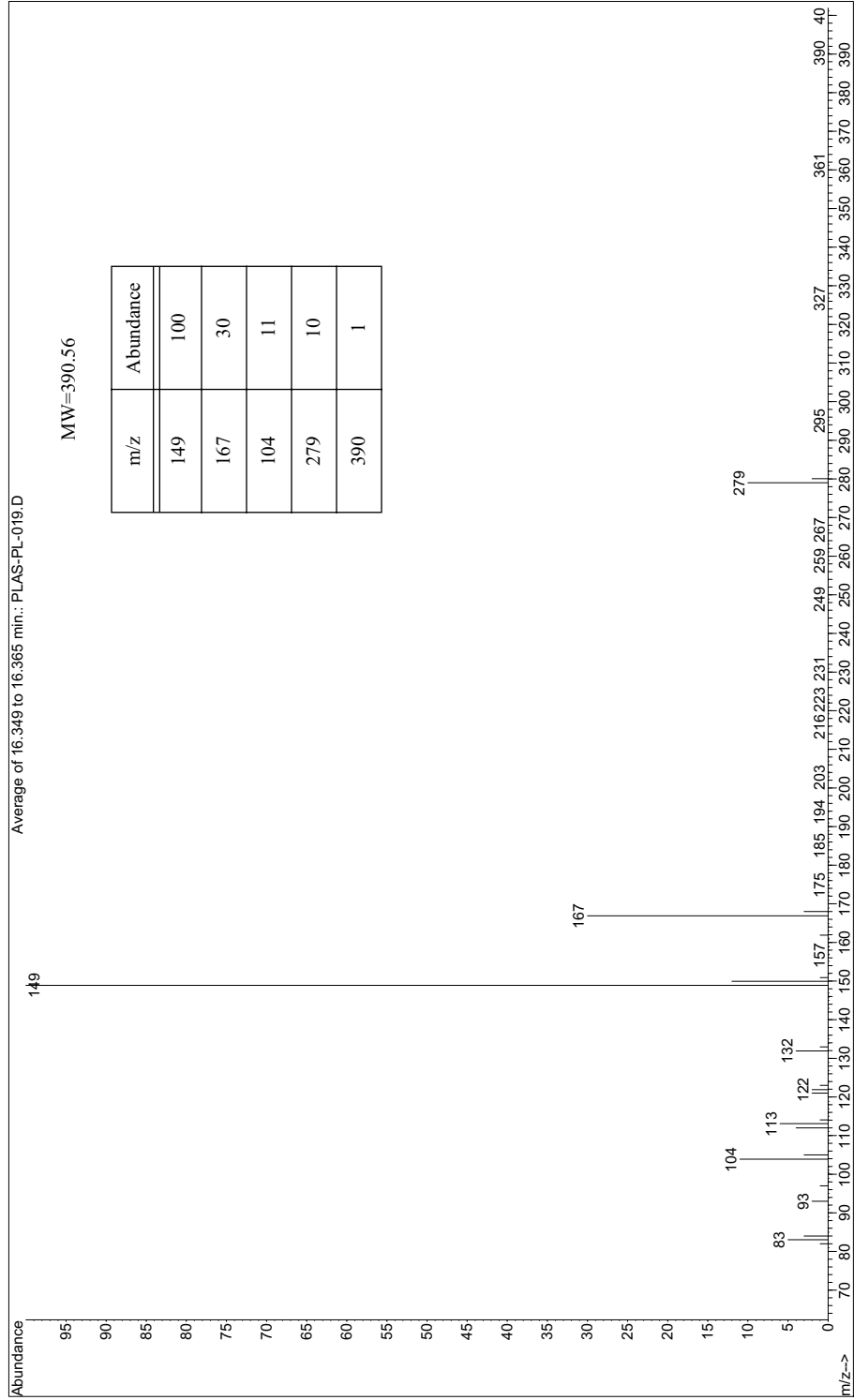
Point of Release

The primary routes of potential human exposure to DOP are air inhalation, ingestion, and dermal contact. For the general population, the most likely route of exposure is through contaminated food (i.e., food coming in contact with containers and wrappings containing this material). It has been detected in such foods as milk, cheese, fish, meat, margarine, eggs, and cereal products. Another potential source of exposure is the leaching of the chemical from plastic articles in landfills.

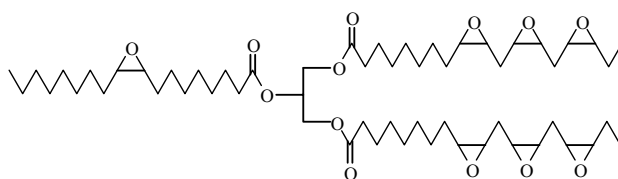
Toxicological Data

Acute oral toxicity (LD50): 30 g/kg [Rat], acute dermal toxicity (LD50): 4 g/kg [Rat]. Listed by NTP as an anticipated human carcinogen and IARC as a possible human carcinogen. Also listed on CA Prop 65 as a known carcinogen.

Mass Spectrum for Dioctyl phthalate (DOP) - PLAS-PL-019



For Chromatogram See Appendix A - PLAS-PL-019 - page 563

Epoxidized linseed oil**CAS Number** 8016-11-3**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₅₇H₉₅O₁₃**Molecular Weight** 1037.39**Chemical Name**

linseed oil, epoxidized

Synonyms

epoxidized linseed oil

Brand Names & Manufacturers

Sold as bulk chemical

Varied

Physical Properties**Appearance** Liquid**Melting Point** -2.2 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.09	U	1-10	1-10	U	1-10

Application, Regulatory & Environmental Information**Application**

Used primarily to keep plastics and rubber soft and pliable in flooring, upholstery, food packaging, hoses, tubing, blood bags, and other products. The epoxy functionality provides heat and light stability.

Regulatory Information

FDA approved for a wide variety of food contact applications.

Environmental Impact

Expected to be readily biodegradable. The estimated log Kow value is > 6.2, which indicates a high potential for bioaccumulation; however, their uptake into fish is expected to be hindered by their large molecular size. If taken up by fish, these carboxylate ester-containing substances are expected to be readily metabolized and excreted. Thus, the bioaccumulation potential is expected to be much lower than predicted from log Kow alone.

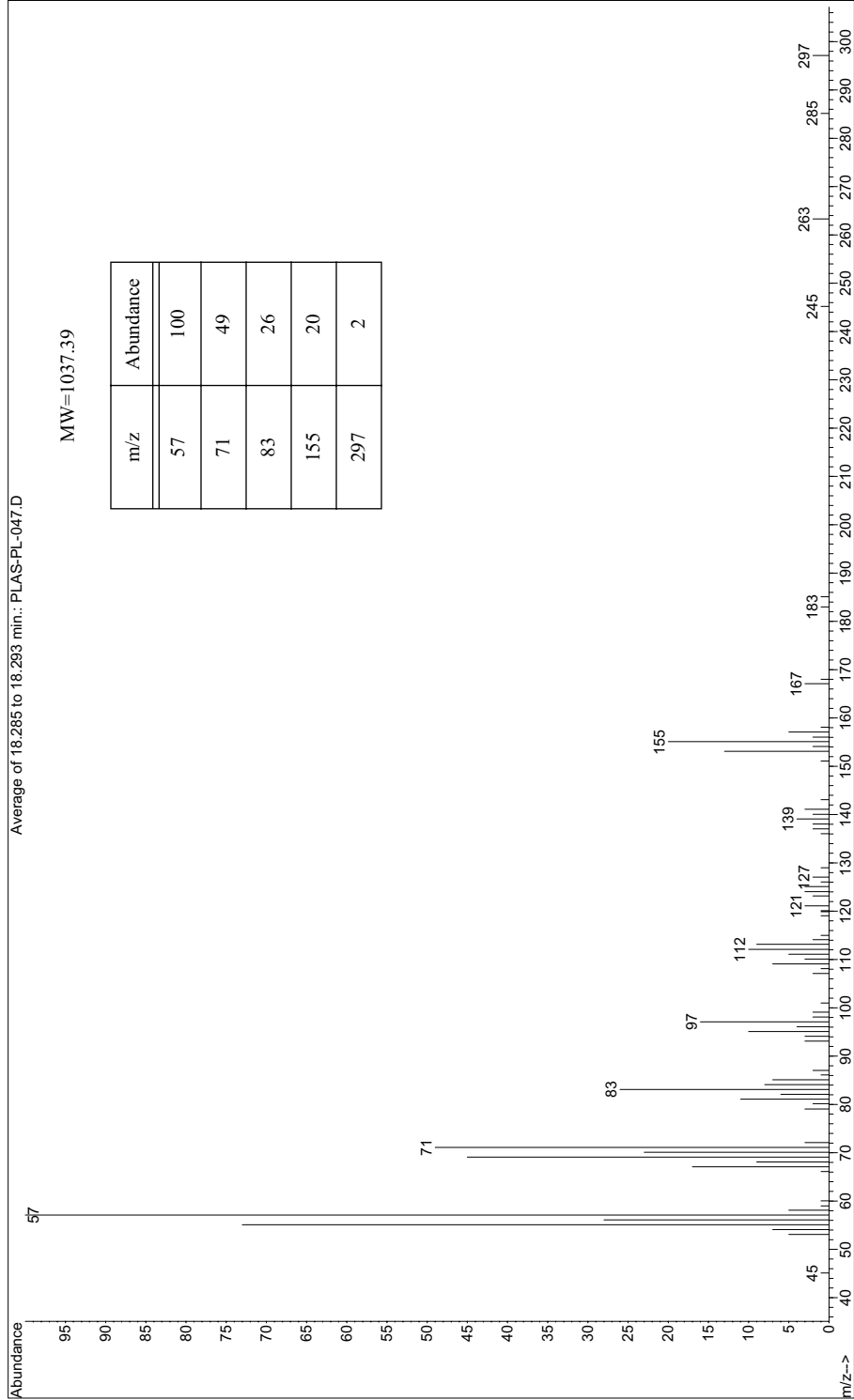
Point of Release

There may be low level losses in process waters, which are discharged to a waste water treatment system. Environmental release during transport is possible in the event of a spill or accident. The material has a very low vapor pressure, making airborne release very unlikely. Migration does occur from plastics during use and upon disposal.

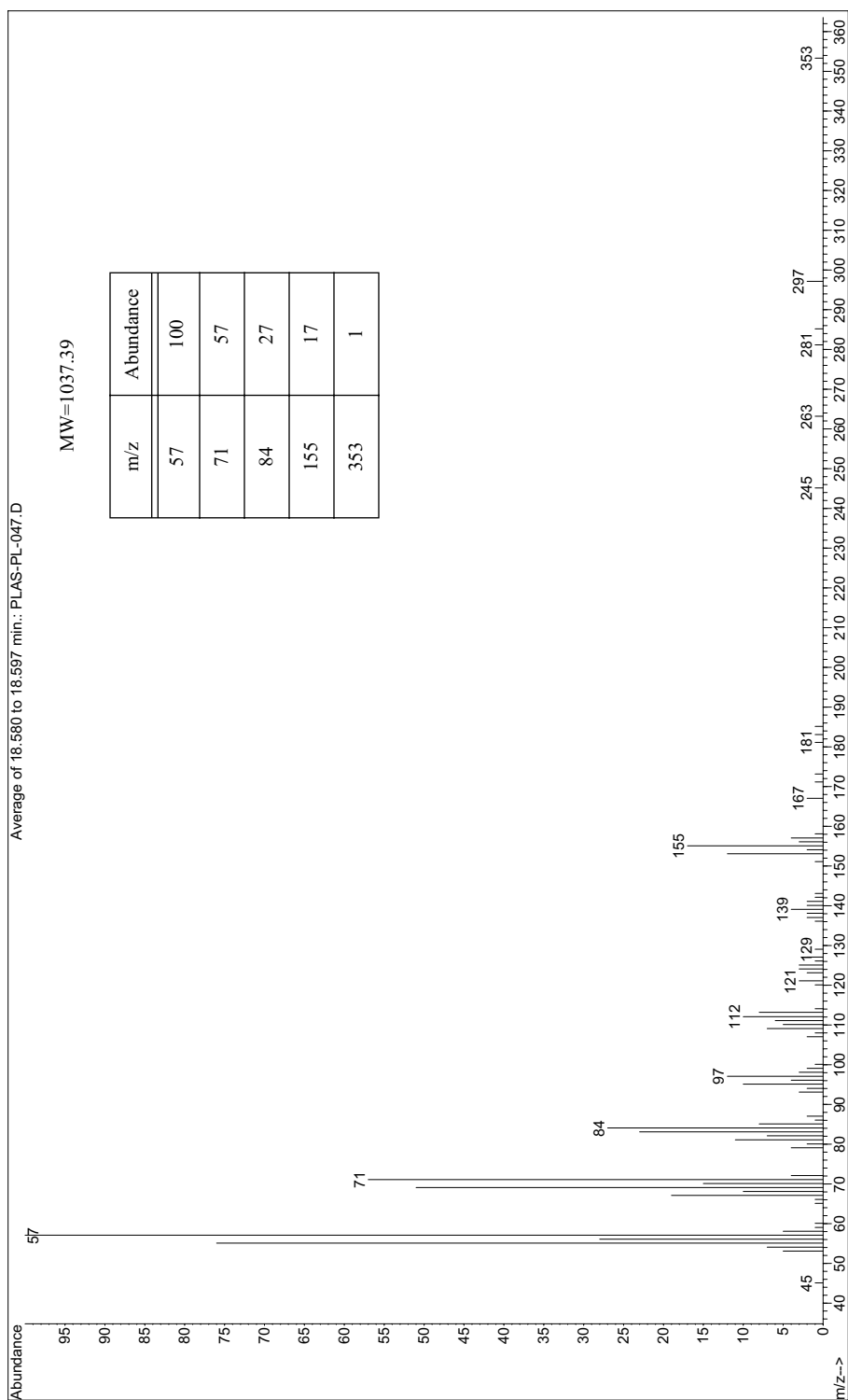
Toxicological Data

While there is no specific information on the metabolism of these materials, there is a large body of research on the metabolism and absorption of vegetable oils. Because of the similarity in physicochemical properties of these materials, it is assumed that they are absorbed and metabolized in a manner similar to vegetable oils, rather than simply excreted.

Mass Spectrum for Epoxidized linseed oil - PLAS-PL-047

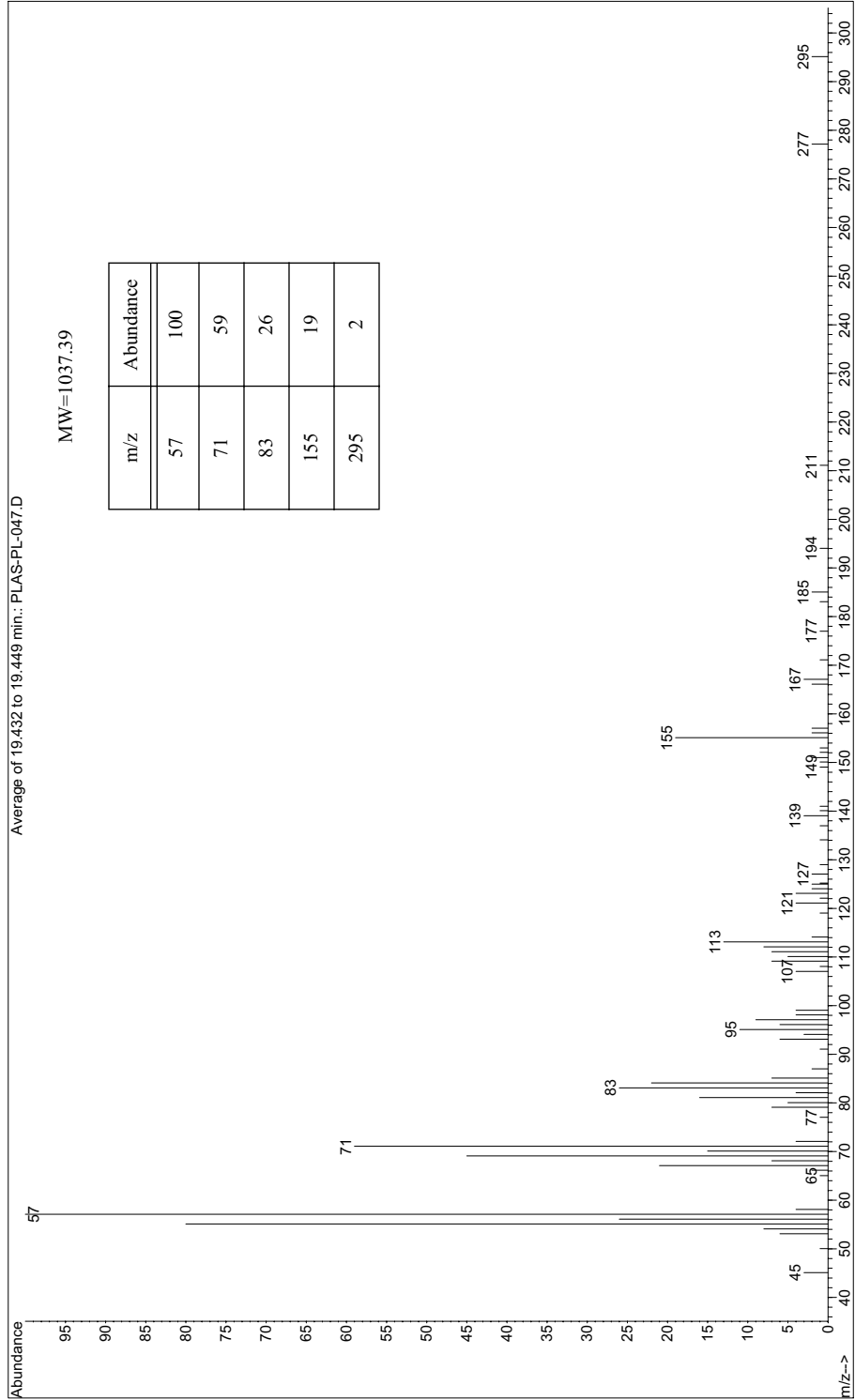


For Chromatogram See Appendix A - PLAS-PL-047 - page 564

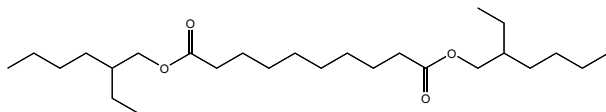
Mass Spectrum for Epoxidized linseed oil - PLAS-PL-047

For Chromatogram See Appendix A - PLAS-PL-047 - page 564

Mass Spectrum for Epoxidized linseed oil - PLAS-PL-047



For Chromatogram See Appendix A - PLAS-PL-047 - page 564

2-Ethylhexyl sebacate**CAS Number** 122-62-3**RTECS Number** VS1000000**Abbreviation** DOS**Formula** C₂₆H₅₀O₄**Molecular Weight** 426.67**Chemical Name**

bis(2-ethylhexyl) decanedioate

Synonyms

dioctyl sebacate

Brand Names & Manufacturers

Monoplex® DOS

HallStar

Physical Properties**Appearance** Straw-colored liquid**Melting Point** -55 °C**Boiling Point** 450-480 °C**Stability** Stable under normal conditions of use.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.01	S	S	U	U	U

Application, Regulatory & Environmental Information

Application Mainly used in polyvinyl chloride, chloroethylene copolymer, nitrocellulose, ethyl cellulose, and synthetic rubber. It is especially suitable material for making cold-resistant cables, leatherette, thin film, and sheet materials. Dioctyl sebacate is often used in combination with acetate o-phthalate plasticizer and can also be used as a plasticizing agent in producing many kinds of synthetic rubbers.

Regulatory Information

FDA regulated for use as an indirect food additive at levels up to 5% by weight.

Environmental Impact

Non toxic for environment; biodegradable.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

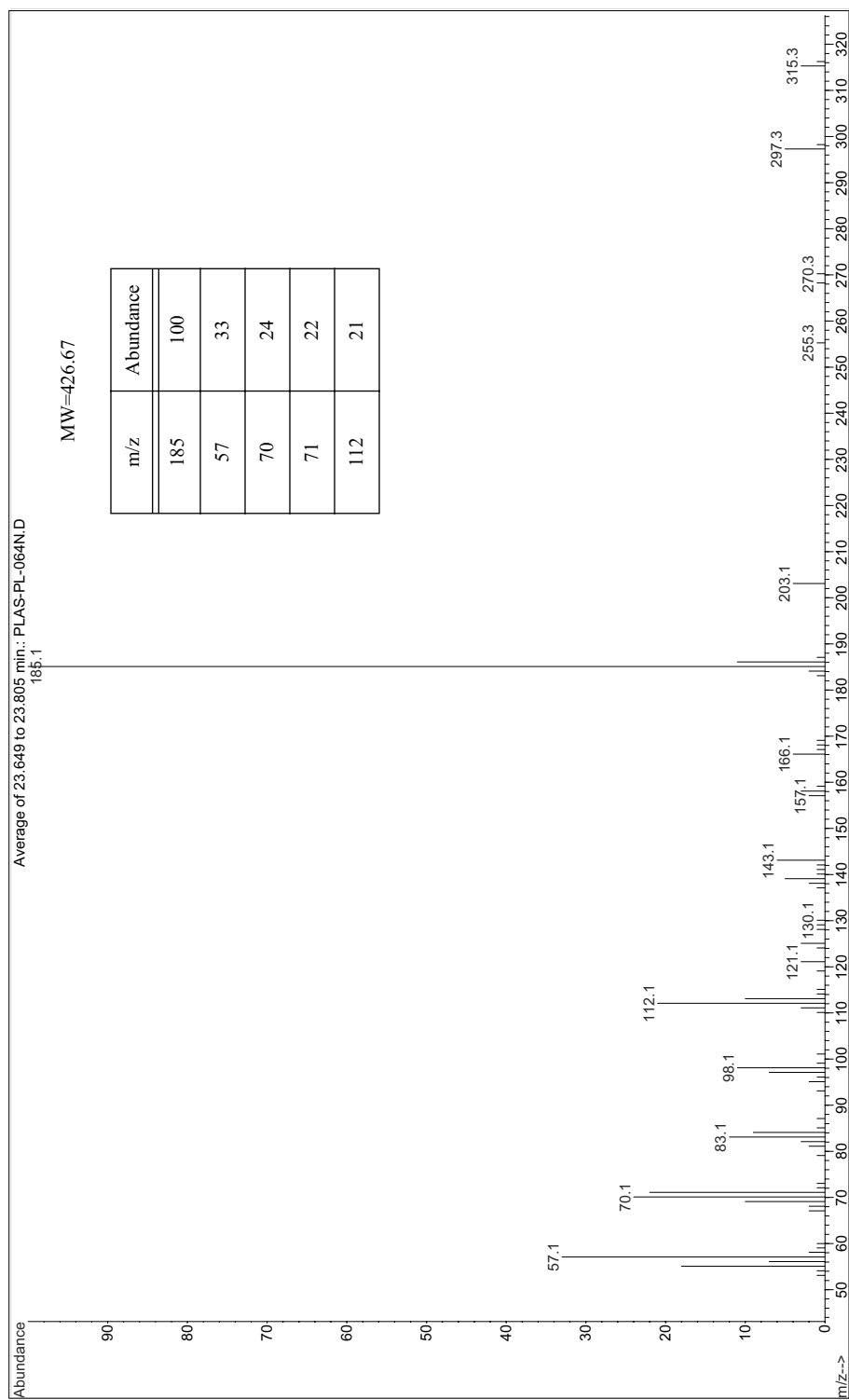
Toxicological Data

Oral: 9500.00 mg/kg [Mouse].

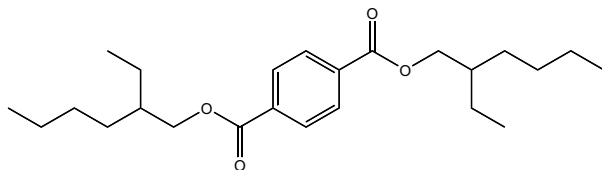
Intravenous: 540.00 mg/kg [Rabbit].

Intravenous: 900.00 mg/kg [Rat].

Mass Spectrum for 2-Ethylhexyl sebacate - PLAS-PL-064



For Chromatogram See Appendix A - PLAS-PL-064 - page 565

bis(2-Ethylhexyl) terephthalate**CAS Number** 6422-86-2**RTECS Number** WZ0883500**Abbreviation** DOTP**Formula** C₂₄H₃₈O₄**Molecular Weight** 390.56**Chemical Name**

bis(2-ethylhexyl) benzene-1,4-dicarboxylate

Synonyms

dioctyl terephthalate; terephthalic acid di-(2-ethylhexyl) ester

Brand Names & Manufacturers

Kodaflex® DOTP

Eastman Chemical

Physical Properties**Appearance** Yellow, viscous liquid**Melting Point** -48 °C**Boiling Point** 400 °C**Stability** Stable under normal conditions of use.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.01	U	S	S	U	U

Application, Regulatory & Environmental Information

Application Used in the manufacture of high temperature cables, automotive plastic parts and components, such as leatherette (artificial leather). Also used in PVC and ABS cements.

Regulatory Information

The toxicity is lower than DOP, but no indication of FDA approval.

Environmental Impact

This product cannot accumulate in living tissue, this product is readily biodegradable in soil and water (speed not given); half-life in air estimated as 18 hours.

Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

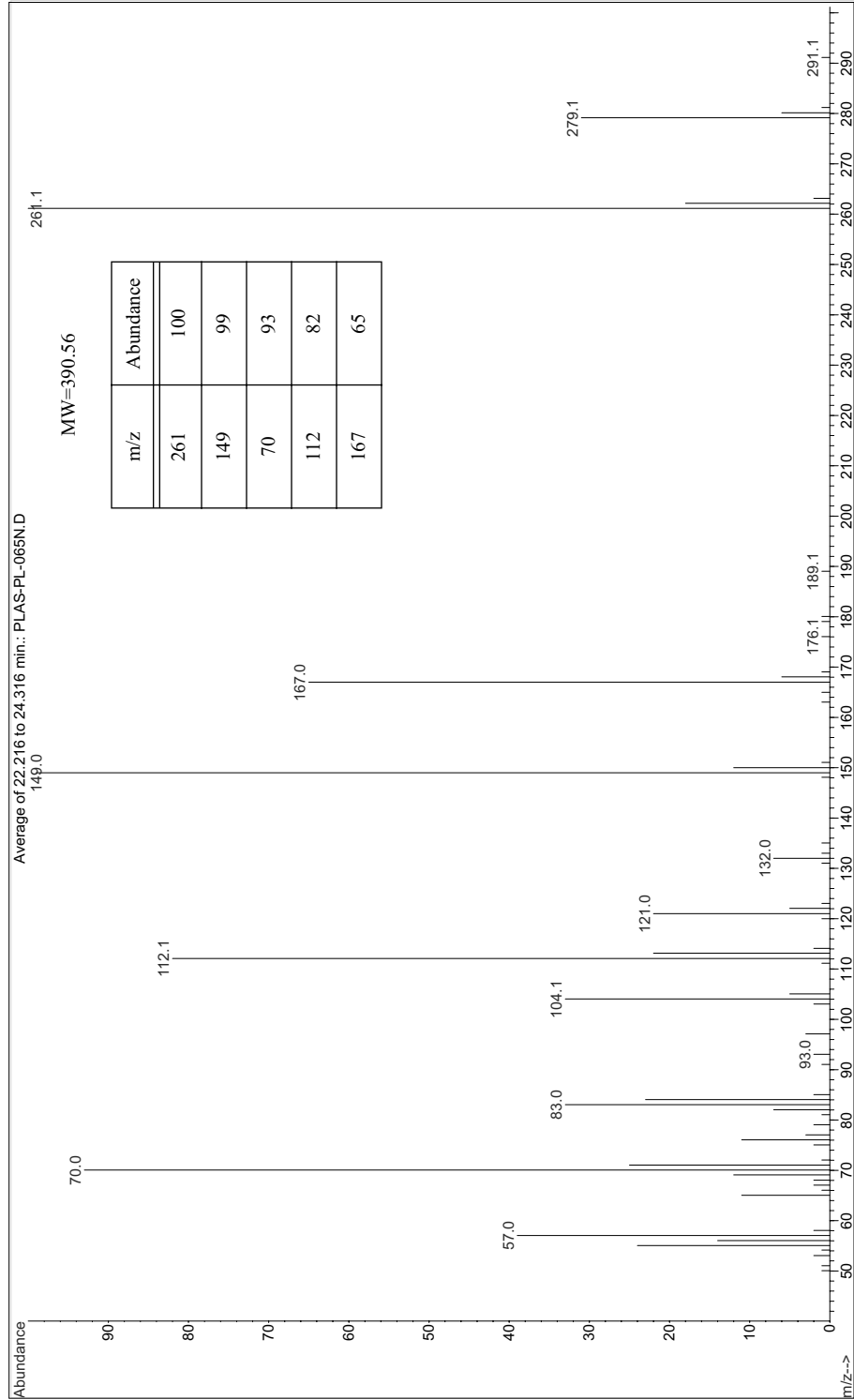
LD50 oral: 20000.

Skin (mg/kg): not known.

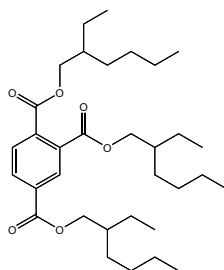
LC50 ppm inhalation: not known.

No known mutagen or reproductive effects in humans or animals.

Mass Spectrum for bis(2-Ethylhexyl) terephthalate - PLAS-PL-065



For Chromatogram See Appendix A - PLAS-PL-045 - page 566

Tris(2-ethylhexyl) Trimellitate**CAS Number** 3319-31-1**RTECS Number** DC2080000**Abbreviation** TOTM**Formula** C₃₃H₅₄O₆**Molecular Weight** 546.78**Chemical Name**

1,2,4-benzenetricarboxylic acid, tris(2-ethylhexyl) ester

Synonyms

trioctyl trimellitate; triethylhexyl trimellitate

Brand Names & Manufacturers

Kodaflex® TOTM	Eastman Chemical
Palatinol® TOTM	BASF
Plasthall® TOTM	HallStar

Physical Properties**Appearance** Light yellow liquid**Melting Point** -38 °C**Boiling Point** 283 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	S	S	S	S	S

Application, Regulatory & Environmental Information

Application Especially useful as a plasticizer in applications requiring good elongation retention such as high-temperature PVC wire coatings. Its excellent resistance to soapy water extraction also makes it attractive for use in vinyl film and vinyl coated fabrics. TOTM is often a good substitute for polyester polymeric plasticizers in low volatility applications where improvements in processing are desired.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

Trimellitates are expected to have low mobility in soil. Volatilization of the trimellitates is expected to be moderate. The rate of hydrolysis is negligible to slow. The rate of atmospheric photooxidation is considered moderate. The trimellitates are expected to have low persistence (P1) and low bioaccumulation potential (B1).

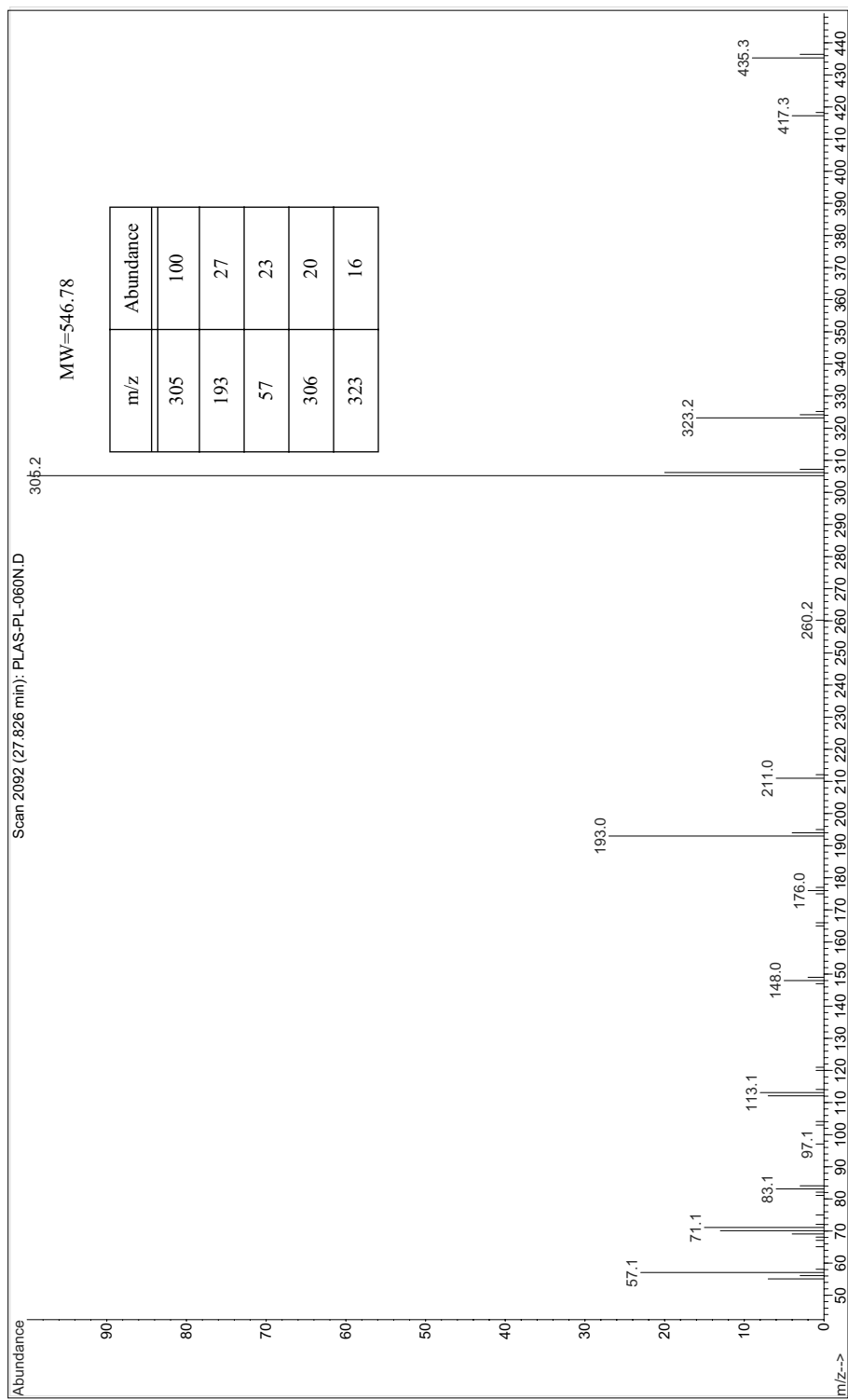
Point of Release

Usually, TOTM is already blended into the compound as a plasticizer, so it is unlikely that downstream users or consumers of electric wire industry, etc. will be exposed to this substance.

Toxicological Data

Repeated exposures via the oral route in rats showed changes in organ weights, clinical chemistry, hematology, and histopathology at 650 mg/kg-bw/day with a NOAEL of 184 mg/kg-bw/day for systemic toxicity. A combined oral reproductive/developmental toxicity screening test in rats showed decreased numbers of spermatocytes and spermatids in the testes at 300 mg/kg-bw/day; the NOAEL for reproductive toxicity was 100 mg/kg-bw/day.

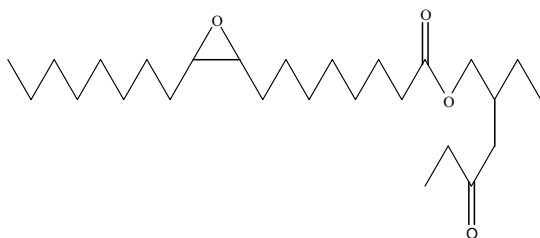
Mass Spectrum for Tris(2-ethylhexyl) Trimellitate - PLAS-PL-060



For Chromatogram See Appendix A - PLAS-PL-060 - page 567

Flexol® EP-8

Houghton Chemical Corporation

**CAS Number** 61789-01-3**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₆H₄₈O₄**Molecular Weight** 424.74**Chemical Name**

fatty acids, tall-oil, epoxidized, 2-ethylhexyl esters

Synonyms

2-ethylhexyl epoxy tallate; expoxidized 2-ethylhexyl ester of tall oil fatty acid; sec-octyl epoxytallate

Brand Names & Manufacturers

Flexol® EP-8

Houghton Chemical Corporation

Physical Properties

Appearance	Liquid					
Melting Point	-23.2 °C			Boiling Point	Decomposes	
Stability	Stable under normal conditions of use.					
Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	0.30	U	1-10	1-10	U	1-10

Application, Regulatory & Environmental Information

Application
Used primarily to keep plastics and rubber soft and pliable in flooring, upholstery, food packaging, hoses, tubing, blood bags, and other products. The epoxy functionality provides heat and light stability.

Regulatory Information

FDA approved for a wide variety of food contact applications.

Environmental Impact

Expected to be readily biodegradable. The estimated log Kow value is > 6.2, which indicates a high potential for bioaccumulation; however, their uptake into fish is expected to be hindered by their large molecular size. If taken up by fish, these carboxylate ester-containing substances are expected to be readily metabolized and excreted. Thus, the bioaccumulation potential is expected to be much lower than predicted from log Kow alone.

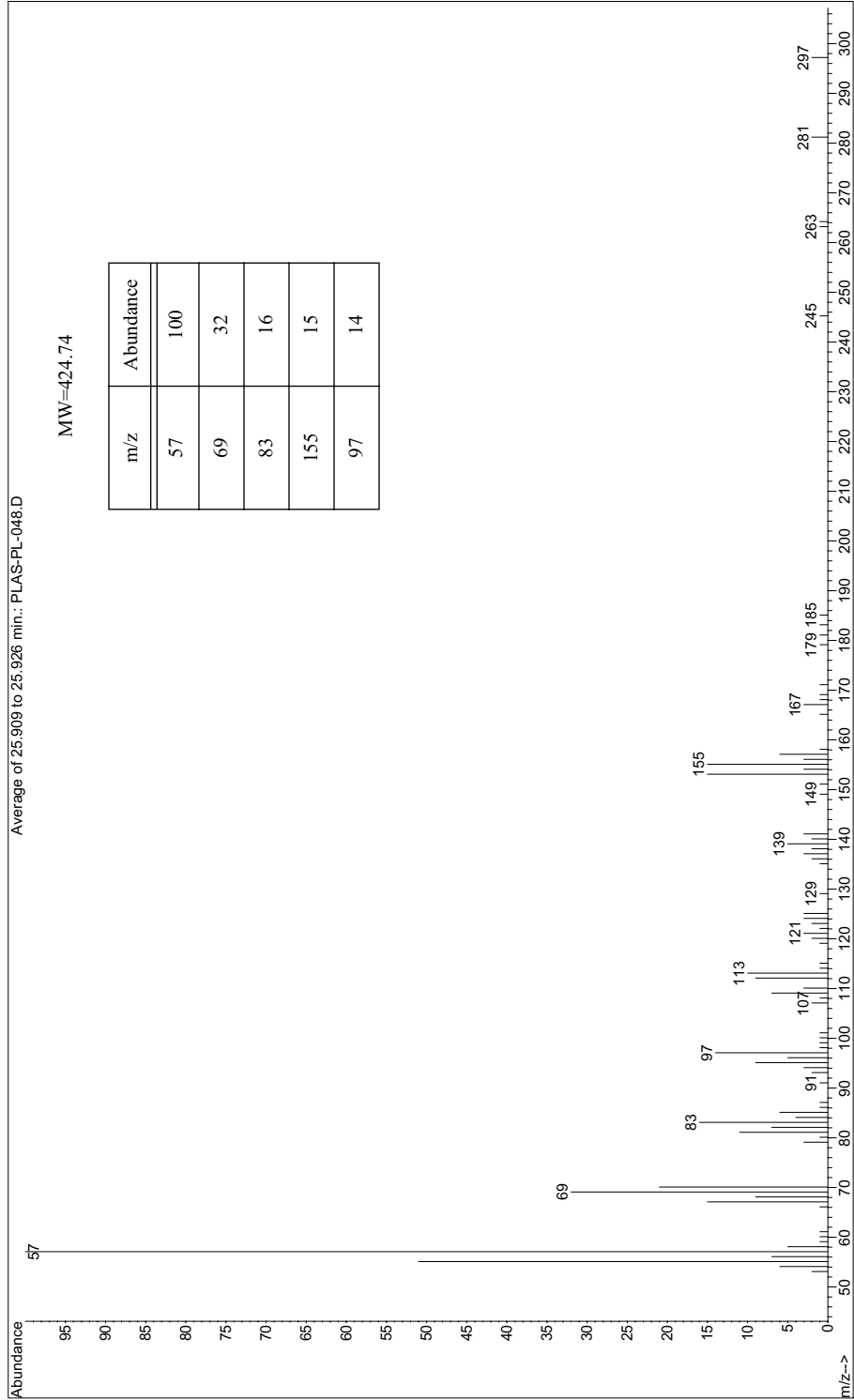
Point of Release

There may be low level losses in process waters, which are discharged to a waste water treatment system. Environmental release during transport is possible in the event of a spill or accident. The material has a very low vapor pressure, making airborne release very unlikely. Migration does occur from plastics during use and upon disposal.

Toxicological Data

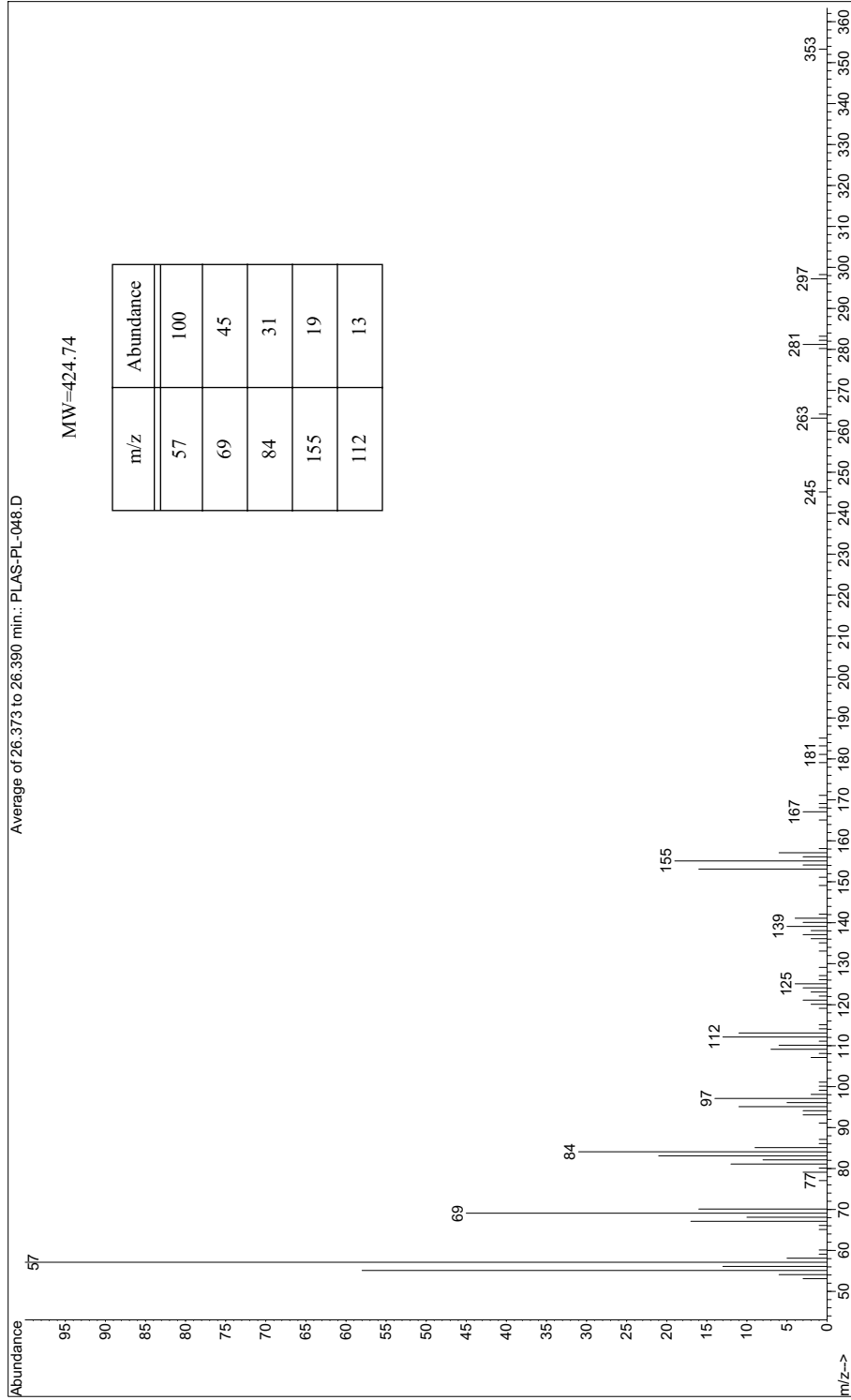
While there is no specific information on the metabolism of these materials, there is a large body of research on the metabolism and absorption of vegetable oils. Because of the similarity in physicochemical properties of these materials, it is assumed that they are absorbed and metabolized in a manner similar to vegetable oils, rather than simply excreted.

Mass Spectrum for Flexol® EP-8 - PLAS-PL-048



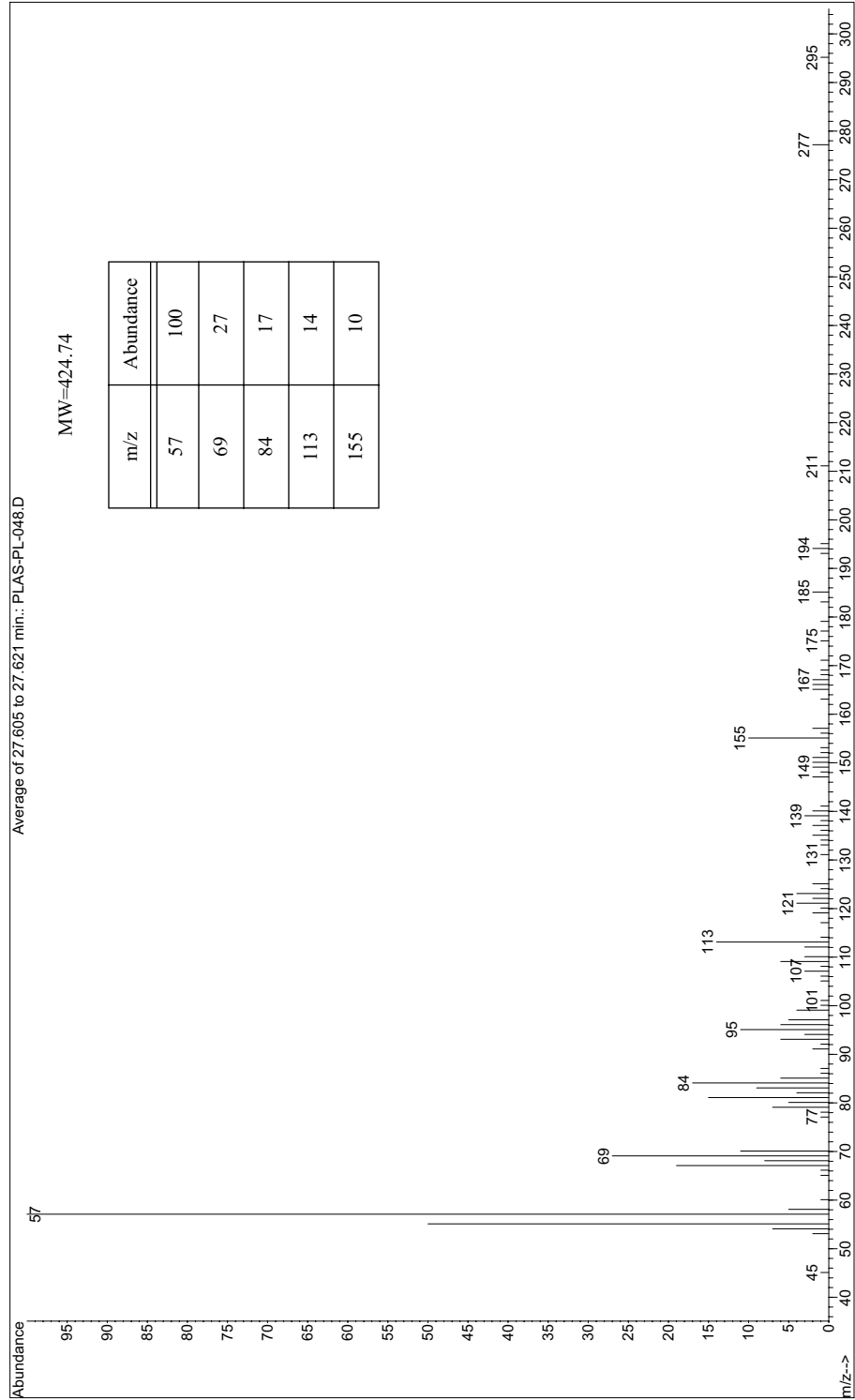
For Chromatogram See Appendix A - PLAS-PL-048 - page 568

Mass Spectrum for Flexol® EP-8 - PLAS-PL-048



For Chromatogram See Appendix A - PLAS-PL-048 - page 568

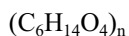
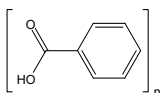
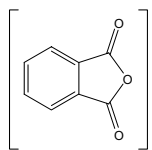
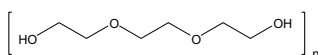
Mass Spectrum for Flexol® EP-8 - PLAS-PL-048



For Chromatogram See Appendix A - PLAS-PL-048 - page 568

Hercoflex® 900

Hercules Incorporated

**CAS Number** 68186-30-1**RTECS Number** N/A**Abbreviation** Not Identified**Formula** See below structure**Molecular Weight** 420.41**Chemical Name**

1,3-isobenzofurandione, polymer with 2,2'-(1,2-ethanediylbis(oxy))bis(ethanol), benzoate

Synonyms

N/A

Brand Names & Manufacturers

Hercoflex 900

Hercules Incorporated

Physical Properties**Appearance** Clear, viscous liquid**Melting Point** Not available**Boiling Point** 197 °C**Stability** Stable under recommended handling and storage conditions.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	40-80	U	U	U	U	U

Application, Regulatory & Environmental Information

Application Plasticizer and adhesion promoter for polyvinyl acetate and other film-formers. Component in latex adhesives, paints, emulsion waxes, polishes, carpet backing, and a variety of other formulations.

Regulatory Information

Approved by the FDA as a food contact additive by 21CFR175.105.

Environmental Impact

Listed as persistent, non-bioaccumulative and not inherently toxic to fish and aquatic organisms.

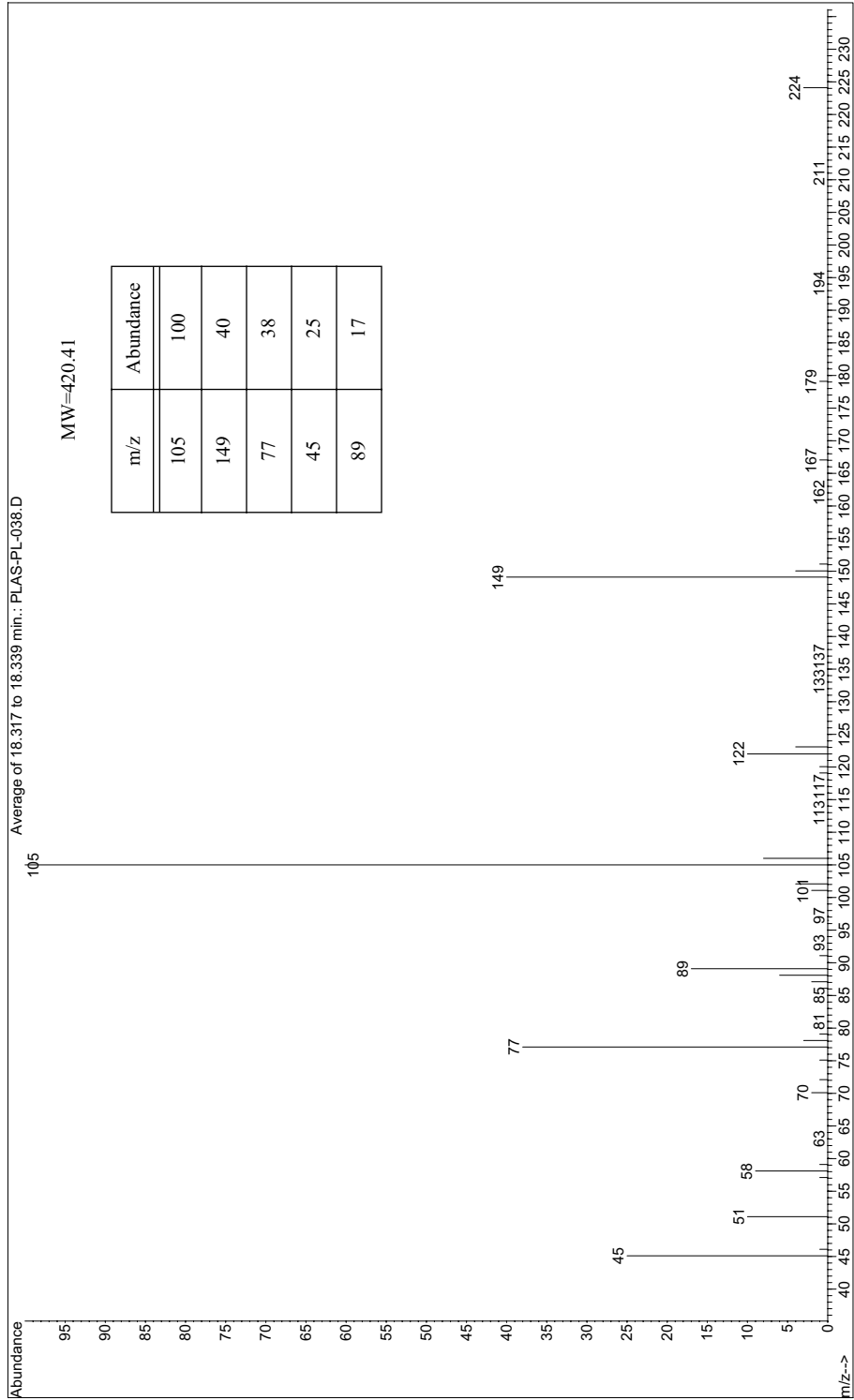
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

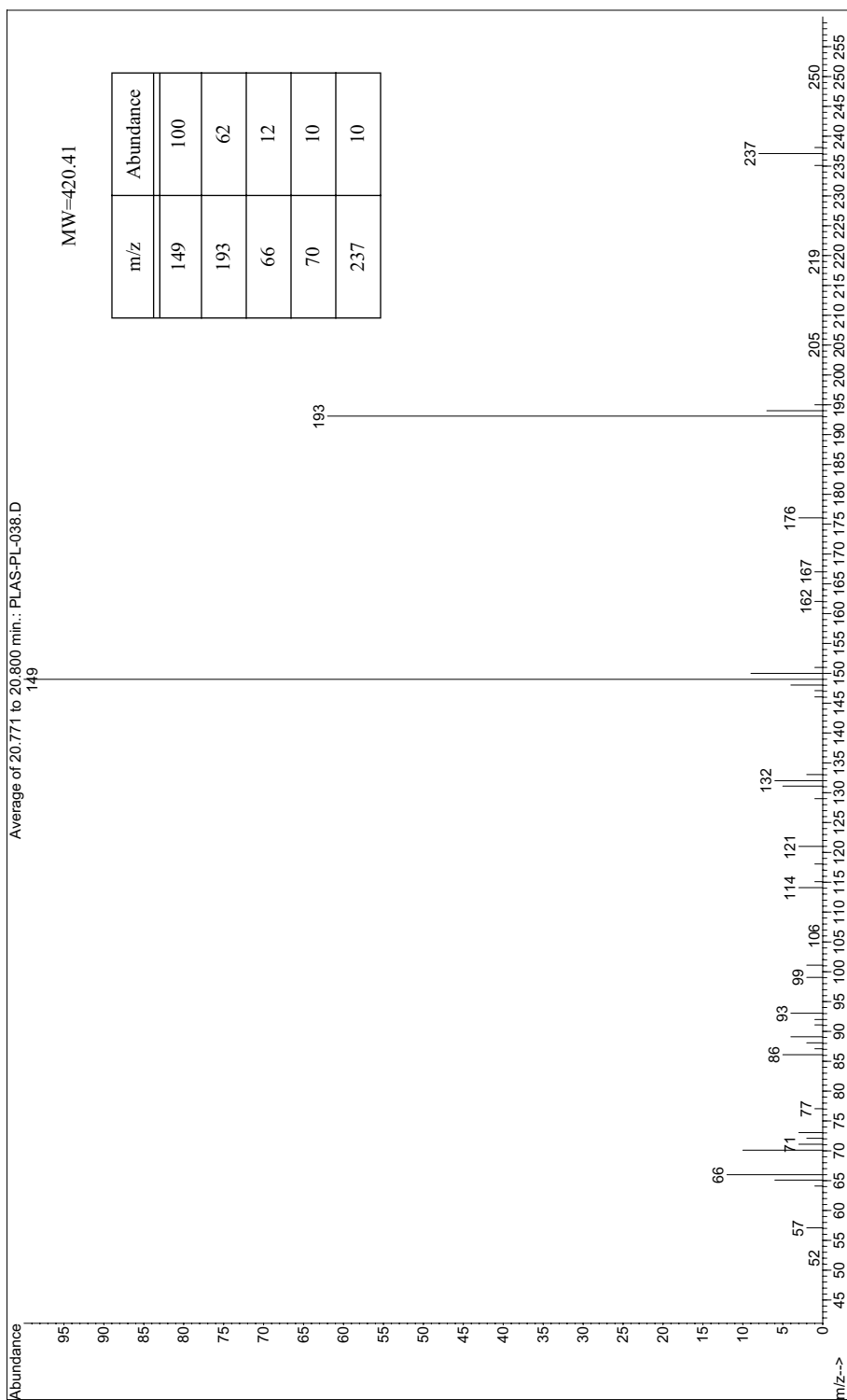
Toxicological Data

Acute oral (LD50): 7.9 g/kg [Rat].

Mass Spectrum for Hercoflex® 900 - PLAS-PL-038

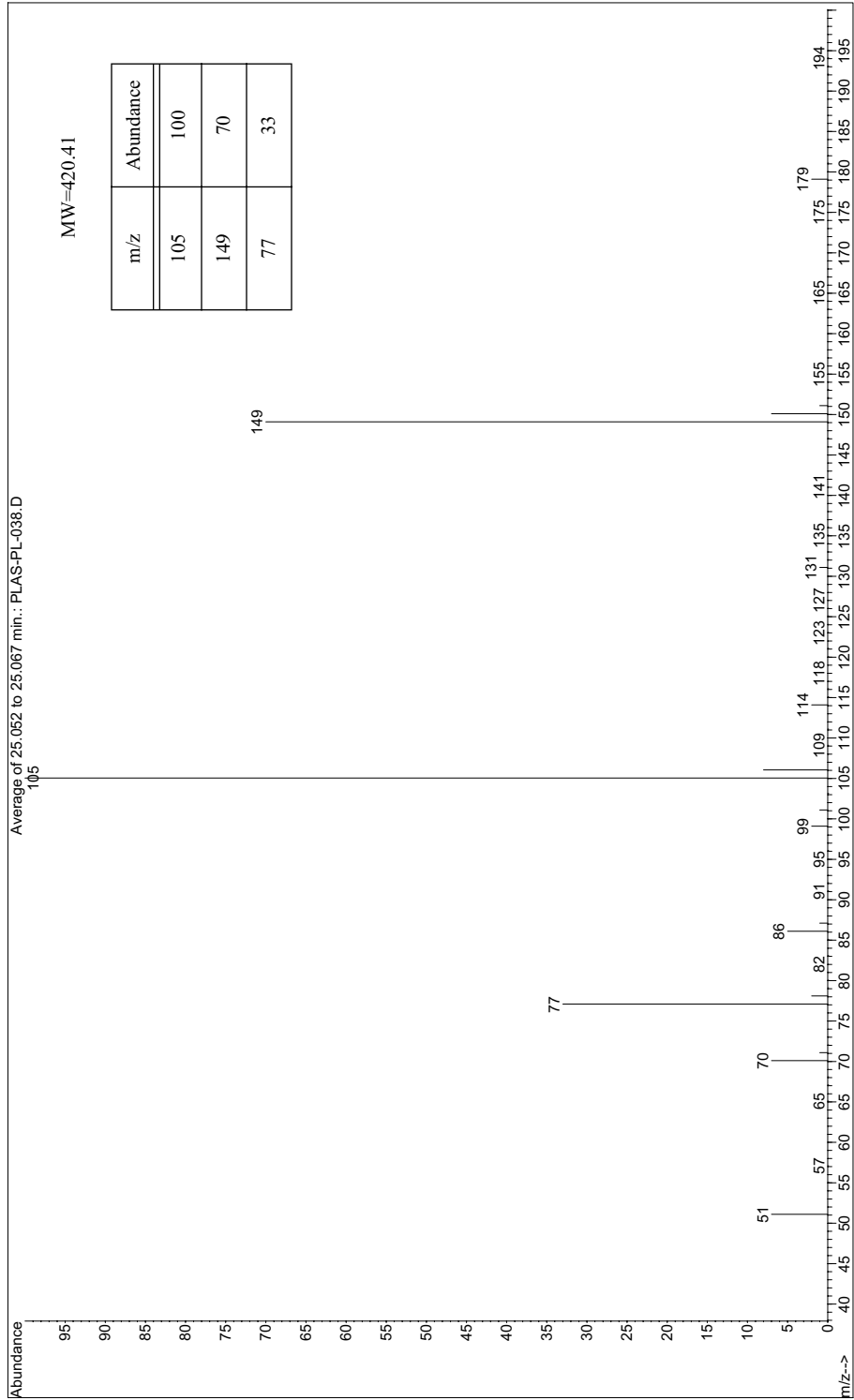


For Chromatogram See Appendix A - PLAS-PL-038 - page 569

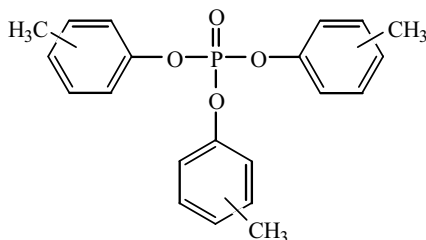
Mass Spectrum for Hercoflex® 900 - PLAS-PL-038

For Chromatogram See Appendix A - PLAS-PL-038 - page 569

Mass Spectrum for Hercoflex® 900 - PLAS-PL-038



For Chromatogram See Appendix A - PLAS-PL-038 - page 569

Imol S-140**CAS Number** 1330-78-5**RTECS Number** TD0175000**Abbreviation** TCP**Formula** C₂₁H₂₁O₄P**Molecular Weight** 368.37**Chemical Name**

phosphoric acid, tris(methylphenyl) ester

Synonyms

tricresyl phosphate; tritolyl phosphate; phosphoric acid; tris(methylphenyl) ester

Brand Names & Manufacturers

Flexol Plasticizer TCP

Phosflex 179A

Physical Properties**Appearance** Clear, faintly yellow, viscous odorless liquid**Melting Point** -33 °C**Boiling Point** 420 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	U	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application**

TCP is used as a plasticizer in vinyl plastics, as a flame-retardant, and as an additive to extreme pressure lubricants. The main market for PVC-based products plasticized with organic phosphate esters is in the manufacture of automobile and other motor vehicle interiors in the US.

Regulatory Information

This product is classified as a toxic material for shipping purposes. It is not approved by the FDA for food contact applications.

Environmental Impact

TCP's low water solubility and high adsorption to particulates causes adsorption onto river or lake sediment and soil. Biodegradation in river water is rapid, almost complete within 5 days. Abiotic degradation is slower with a half-life of 96 days. BCFs of 165-2768 were measured for several fish species in the laboratory using radiolabelled TCP. Radioactivity was lost rapidly on cessation of exposure, depuration half-lives ranged between 25.8 and 90 hours.

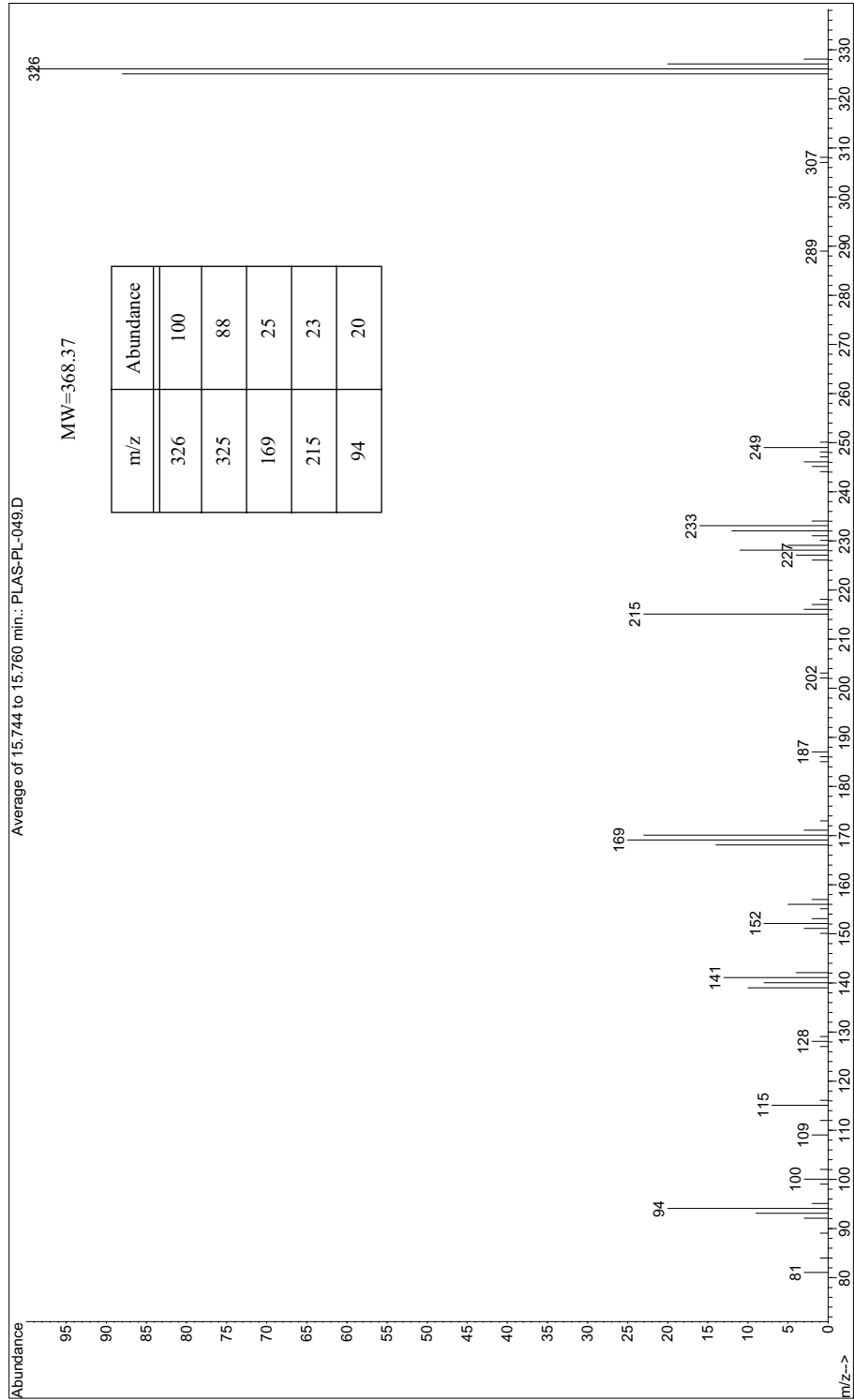
Point of Release

This product can be released into the atmosphere more rapidly in extreme temperatures. In addition, UV exposure from parking in the sun creates a favorable environment for chemical breakdown. The extreme conditions of heat and sunlight in the interior of an automobile can cause gasses to escape from the plasticizer.

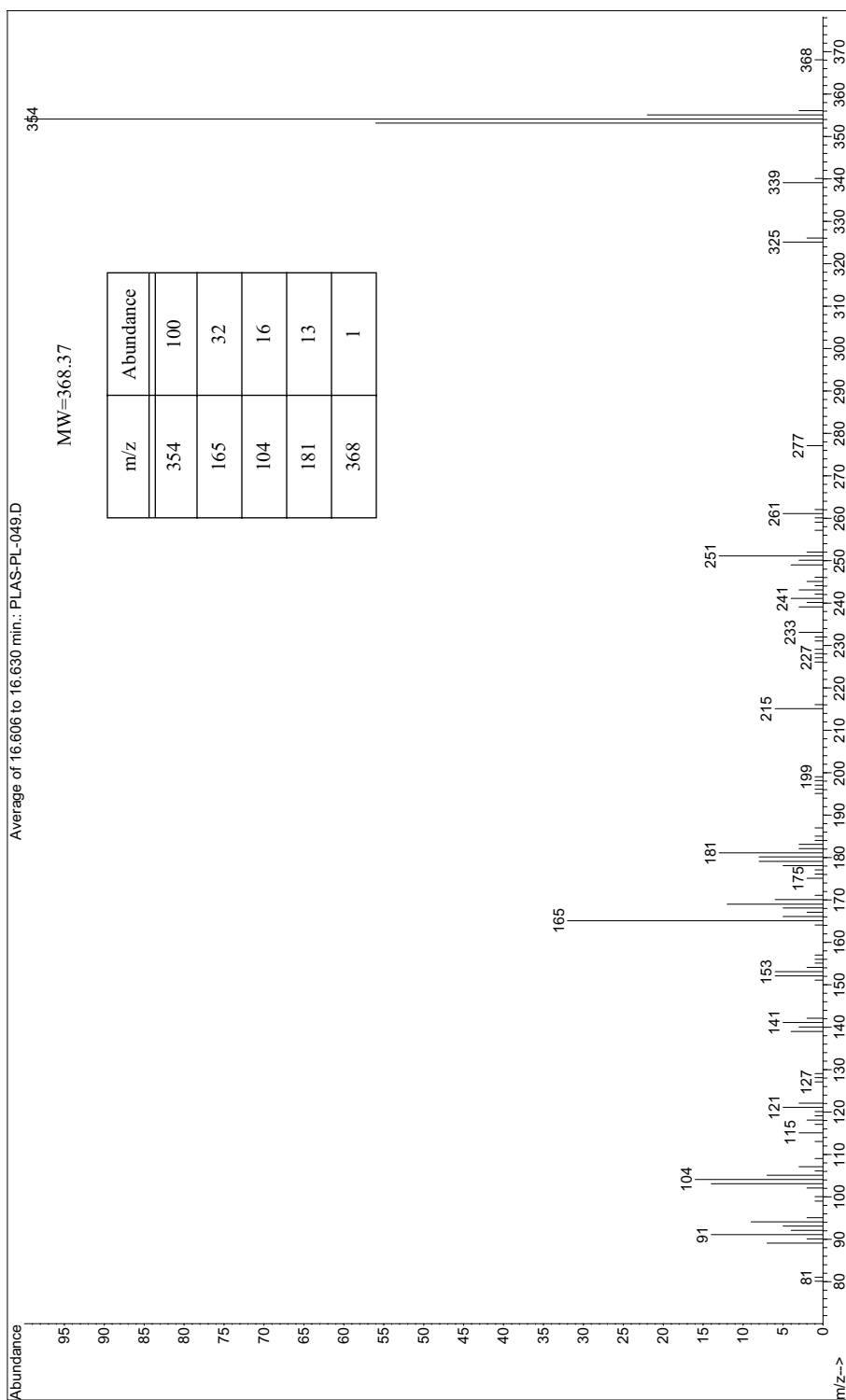
Toxicological Data

This substance is toxic to the central nervous system.

Mass Spectrum for Imol S-140 - PLAS-PL-049

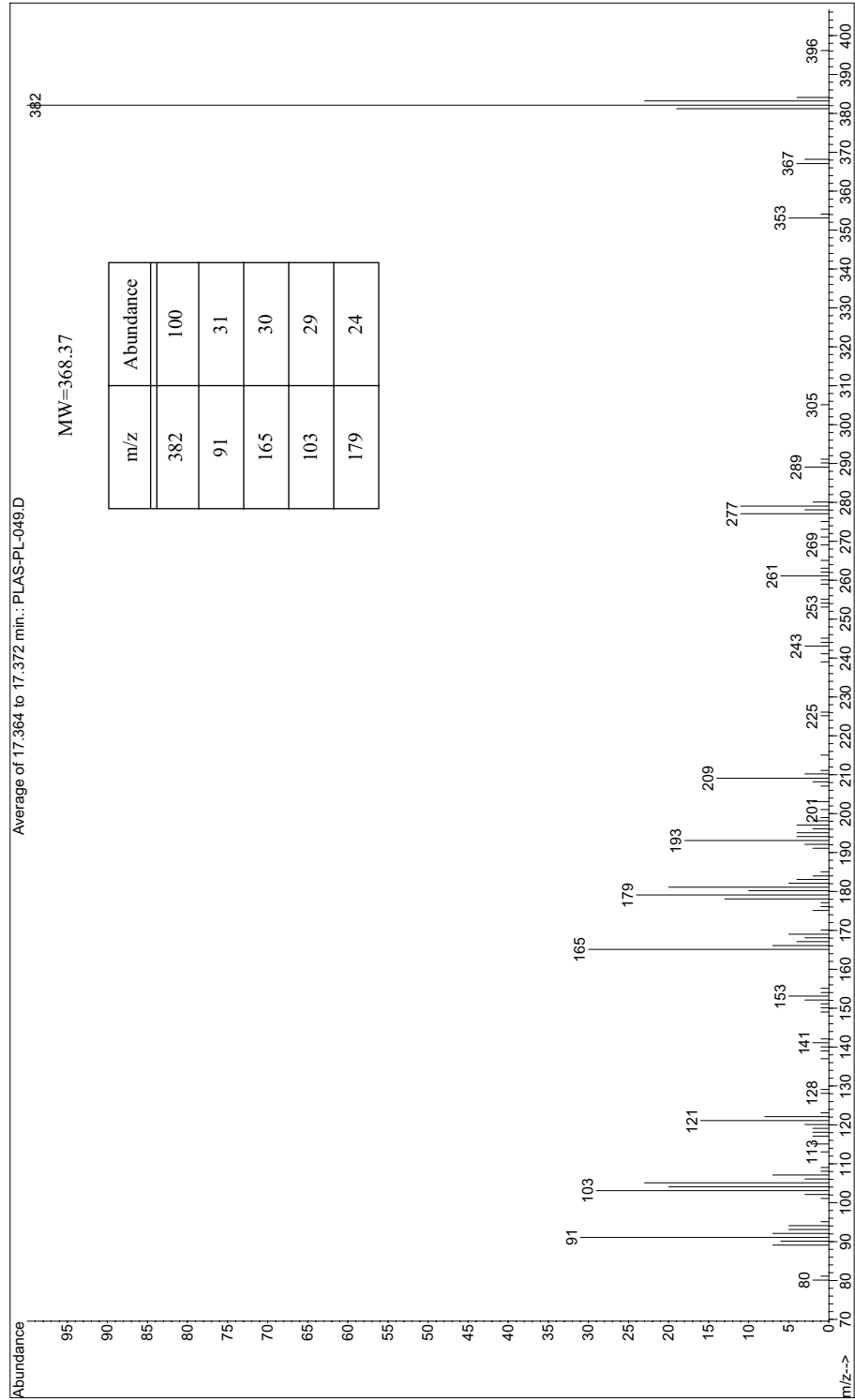


For Chromatogram See Appendix A - PLAS-PL-049 - page 570

Mass Spectrum for Imol S-140 - PLAS-PL-049

For Chromatogram See Appendix A - PLAS-PL-049 - page 570

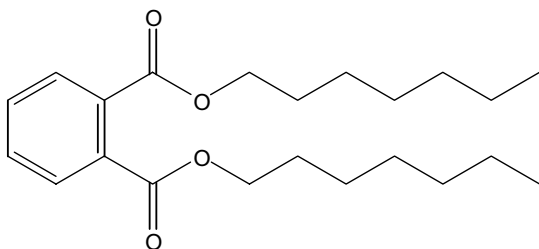
Mass Spectrum for Imol S-140 - PLAS-PL-049



For Chromatogram See Appendix A - PLAS-PL-049 - page 570

Jayflex® 77

ExxonMobil Corporation

**CAS Number** 71888-89-6**RTECS Number** N/A**Abbreviation** DIHP**Formula** C₂₂H₃₄O₄**Molecular Weight** 362.50**Chemical Name**
diisooheptyl phthalate**Synonyms**
1,2-benzenedicarboxylic acid**Brand Names & Manufacturers**

Jayflex 77

ExxonMobil Corporation

Physical Properties

Physical Properties						
Appearance	Clear liquid, characteristic odor					
Melting Point	Not available			Boiling Point >300 °C		
Stability	Stable under normal conditions of use.					
Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.01	U	U	U	U	U

Application **Application, Regulatory & Environmental Information**

Used as a plasticizer for molding and coating plastisols, vinyl flooring, tile, and carpet backing. May also be used as a partial replacement for higher molecular weight phthalate plasticizers (extrusion, injection molding, and calendaring applications).

Regulatory Information

This product does not have FDA approval for food contact applications.

Environmental Impact

Test data indicates no associated acute aquatic toxicity but may show chronic toxicity. It is reported to be readily biodegradable, but may pose a moderate bioaccumulative risk based on a log Kow value of 5.6.

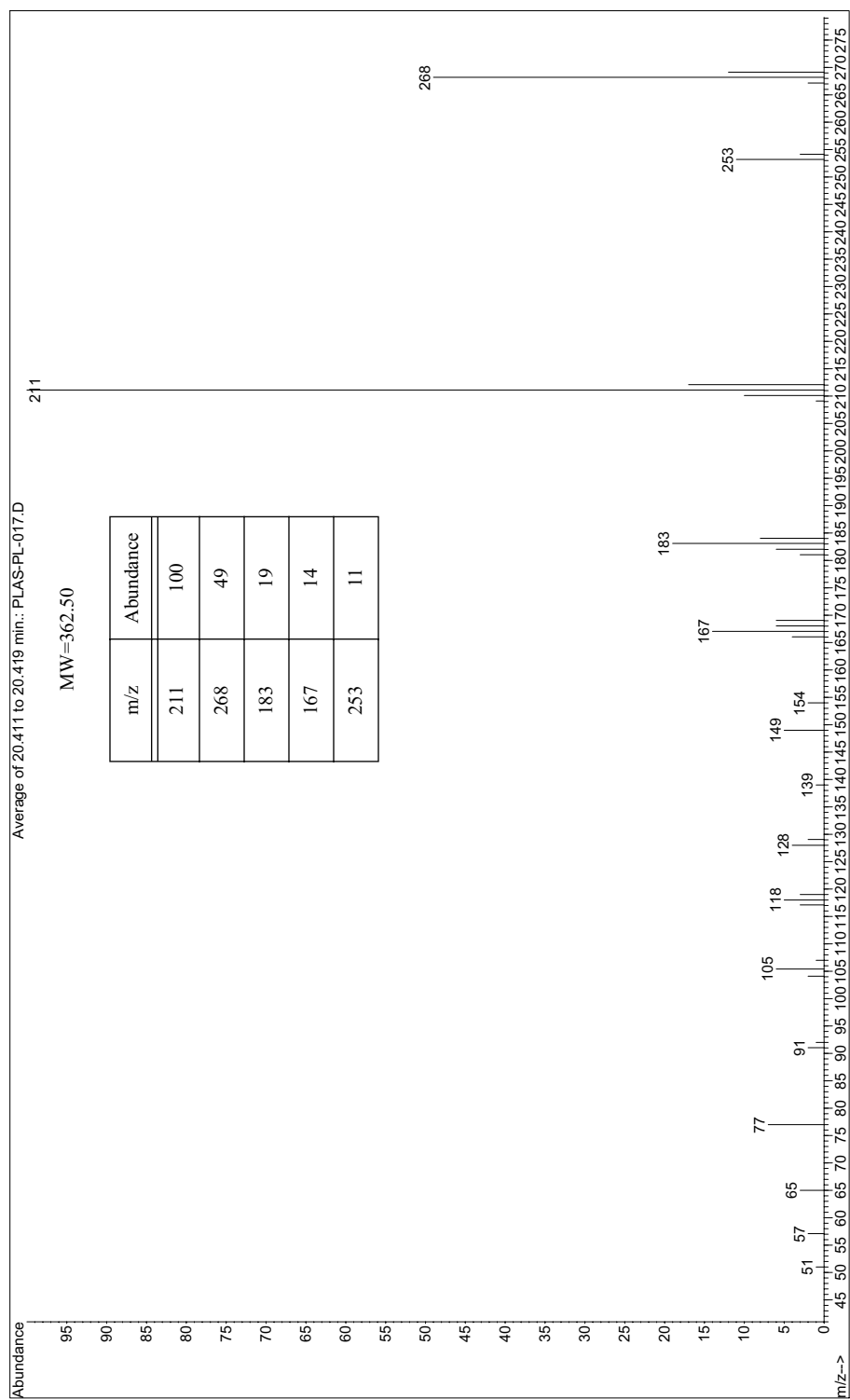
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

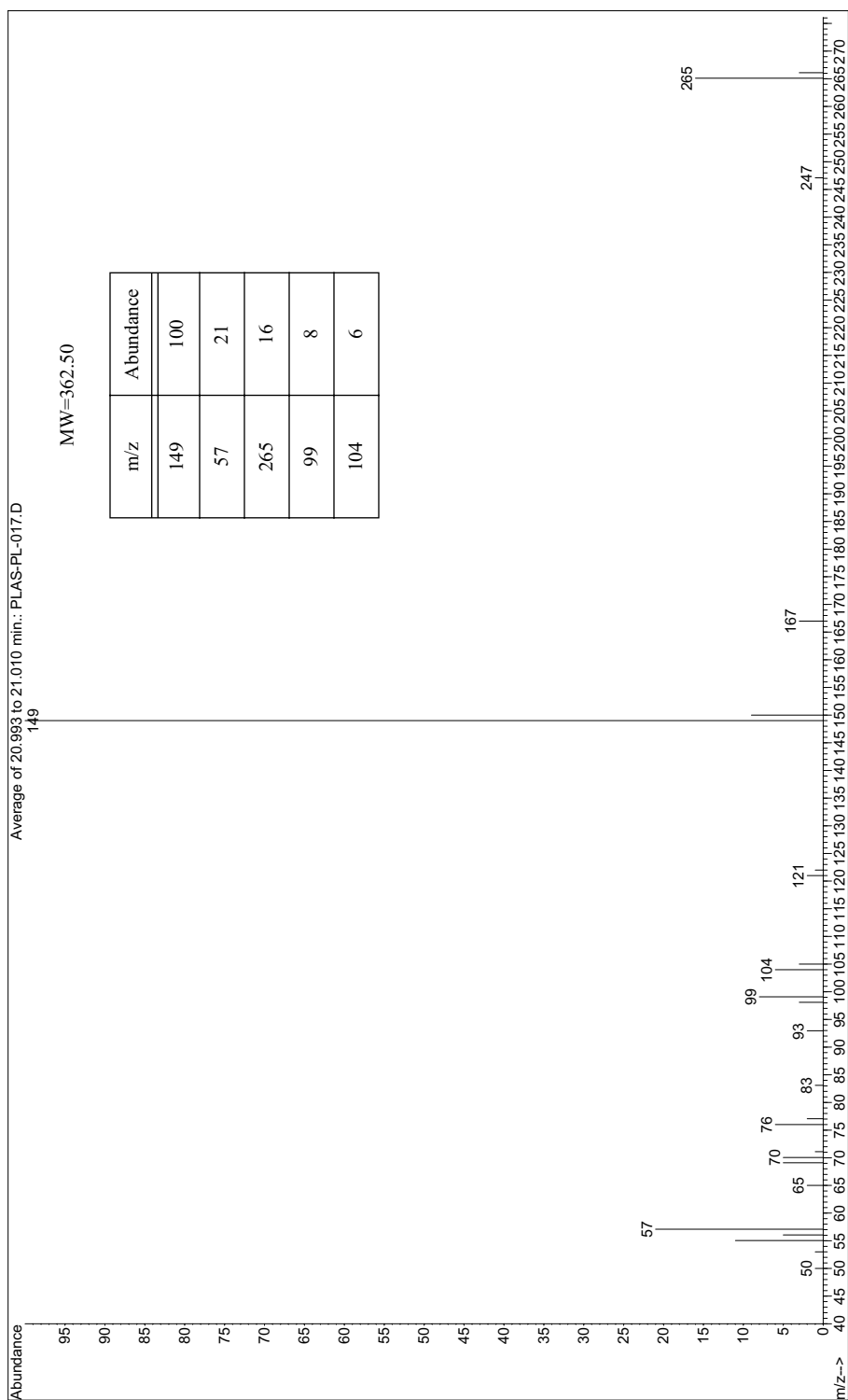
Toxicological Data

This compound is classified as a transitional phthalate, which has greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. It is not listed by ACGIH, IARC, NTP, or OSHA as a cancer causing agent.

Mass Spectrum for Jayflex® 77 - PLAS-PL-017

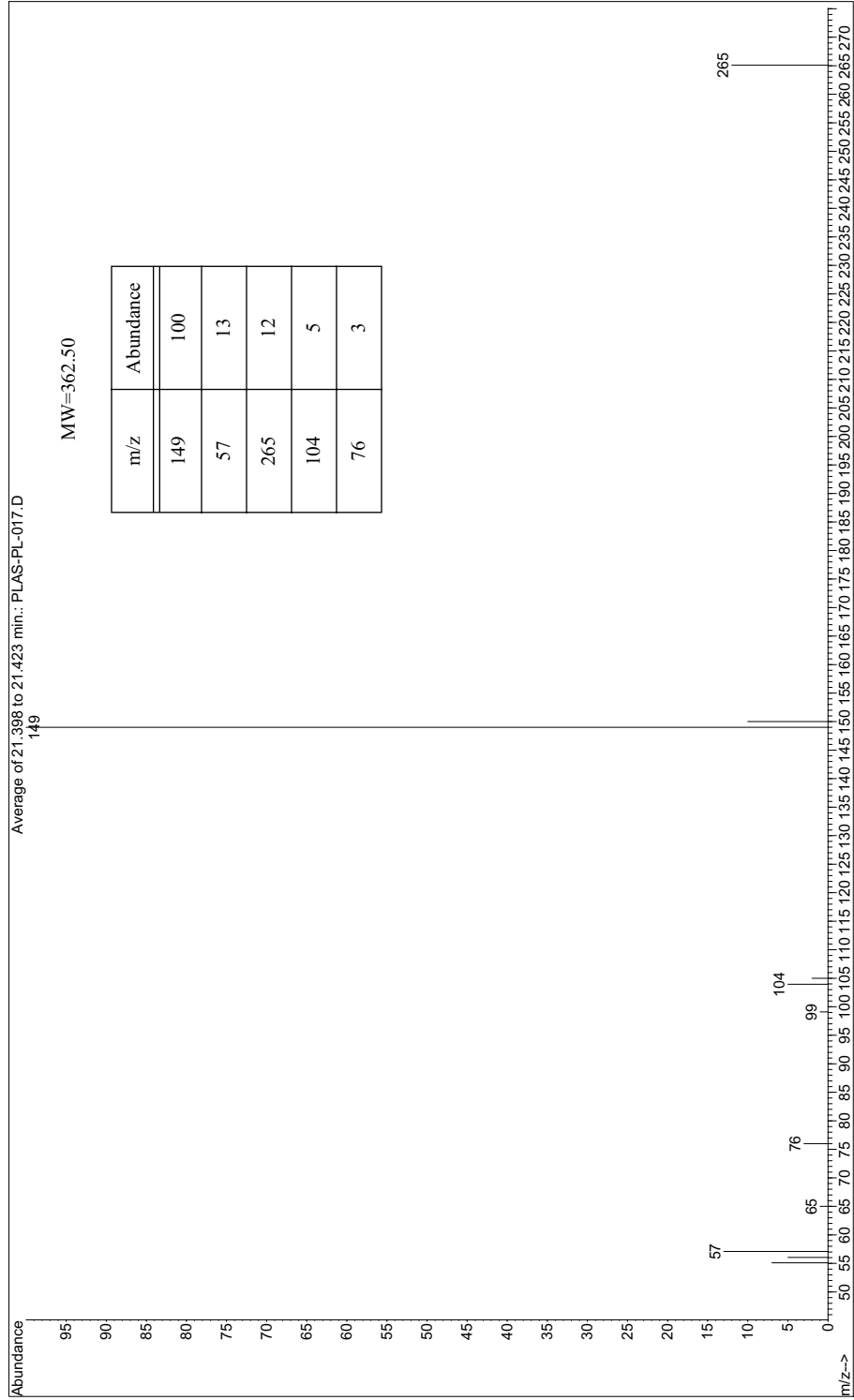


For Chromatogram See Appendix A - PLAS-PL-017 - page 571

Mass Spectrum for Jayflex® 77 - PLAS-PL-017

For Chromatogram See Appendix A - PLAS-PL-017 - page 571

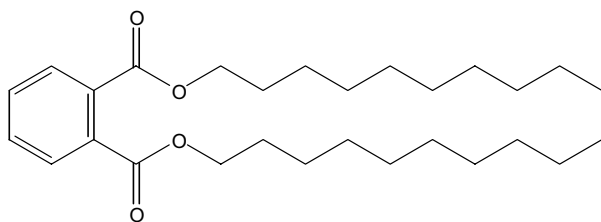
Mass Spectrum for Jayflex® 77 - PLAS-PL-017



For Chromatogram See Appendix A - PLAS-PL-017 - page 571

Jayflex® DIDP

ExxonMobil Corporation

**CAS Number** 68515-49-1**RTECS Number** N/A**Abbreviation** DIDP**Formula** C₂₈H₄₆O₄**Molecular Weight** 446.66**Chemical Name**

diisodecyl phthalate

Synonyms

bis(8-methylnonyl) phthalate; 1,2-benzenedicarboxylic acid diisodecyl ester

Brand Names & Manufacturers

Palatinol® DIDP

BASF

Physical Properties**Appearance** Clear, oily liquid; mild odor**Melting Point** Not available**Boiling Point** 250-257 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application**

DIDP is a general purpose plasticizer with a broad range of applications used in flexible PVC. It is widely used in the toy, construction, automotive, and general consumer product markets. It has limited use in food packaging and is not used in medical applications.

Regulatory Information

Regulated by the State of California Safe Drinking Water Act of 1986.

Environmental Impact

This material is expected to be readily biodegradable and partition to sediment and wastewater solids if released to the environment, but is not expected to be harmful to aquatic organisms. Log Kow value of 8.8 indicates a high potential to bioaccumulate. It is also listed as a persistent bioaccumulative toxin in Europe.

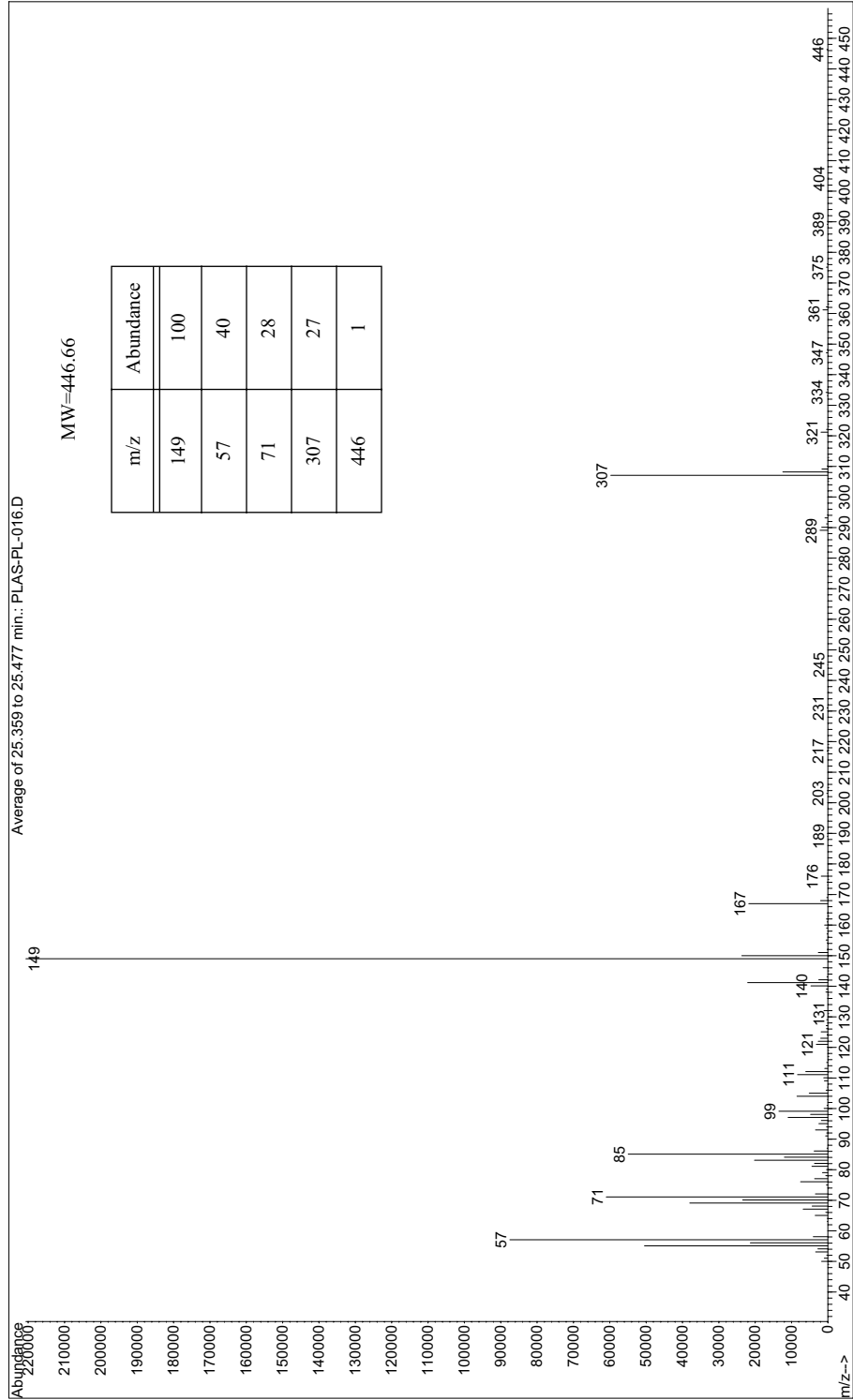
Point of Release

Humans may be exposed to DIDP by the oral, dermal, and inhalation routes of exposure. Occupational exposure occurs primarily through inhalation and dermal contact, while consumer exposure occurs primarily through oral and dermal routes. Exposure of children to DIDP through children's products is a public concern.

Toxicological Data

Not listed (ACGIH, IARC, NTP, OSHA) as a cancer causing agent although it has been shown to cause a small, but statistically significant increased early offspring mortality at high oral doses in a 2-generation reproductive study in laboratory animals. Is on CA Proposition 65 list as a chemical known to the State of California to cause developmental toxicity and reproductive toxicity for purposes of the Safe Drinking Water and Toxic Enforcement Act of 1986.

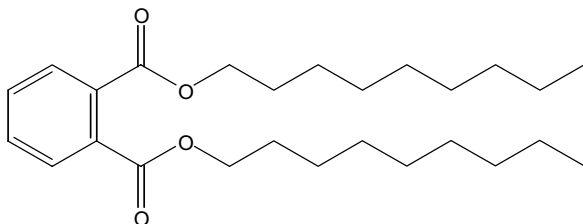
Mass Spectrum for Jayflex® DIDP - PLAS-PL-016



For Chromatogram See Appendix A - PLAS-PL-016 - page 572

Jayflex® DINP

ExxonMobil Corporation

**CAS Number** 68515-48-0**RTECS Number** CZ3395000**Abbreviation** DINP**Formula** C₂₆H₂₂O₄**Molecular Weight** 418.61**Chemical Name**

diisononyl phthalate

Synonyms

1,2 benzenedicarboxylic acid, di-C9-11 branched alkyl ester

Brand Names & Manufacturers

Palatinol® DINP

BASF

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** N/A**Boiling Point** >250 °C**Stability** Stable under normal conditions of use.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.1	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

General purpose branched phthalate plasticizer used in coated fabric, film and sheeting, flooring, injection molding, and profile extrusion and plastisols.

Regulatory Information

Diisononyl phthalate is FDA approved at levels up to 43%.

Environmental Impact

Not expected to be harmful to aquatic organisms. Not expected to demonstrate chronic toxicity to aquatic organisms. Material is expected to partition to sediment and wastewater solids. Minimally volatile. Expected to be readily biodegradable and the potential to bioaccumulate is low.

Point of Release

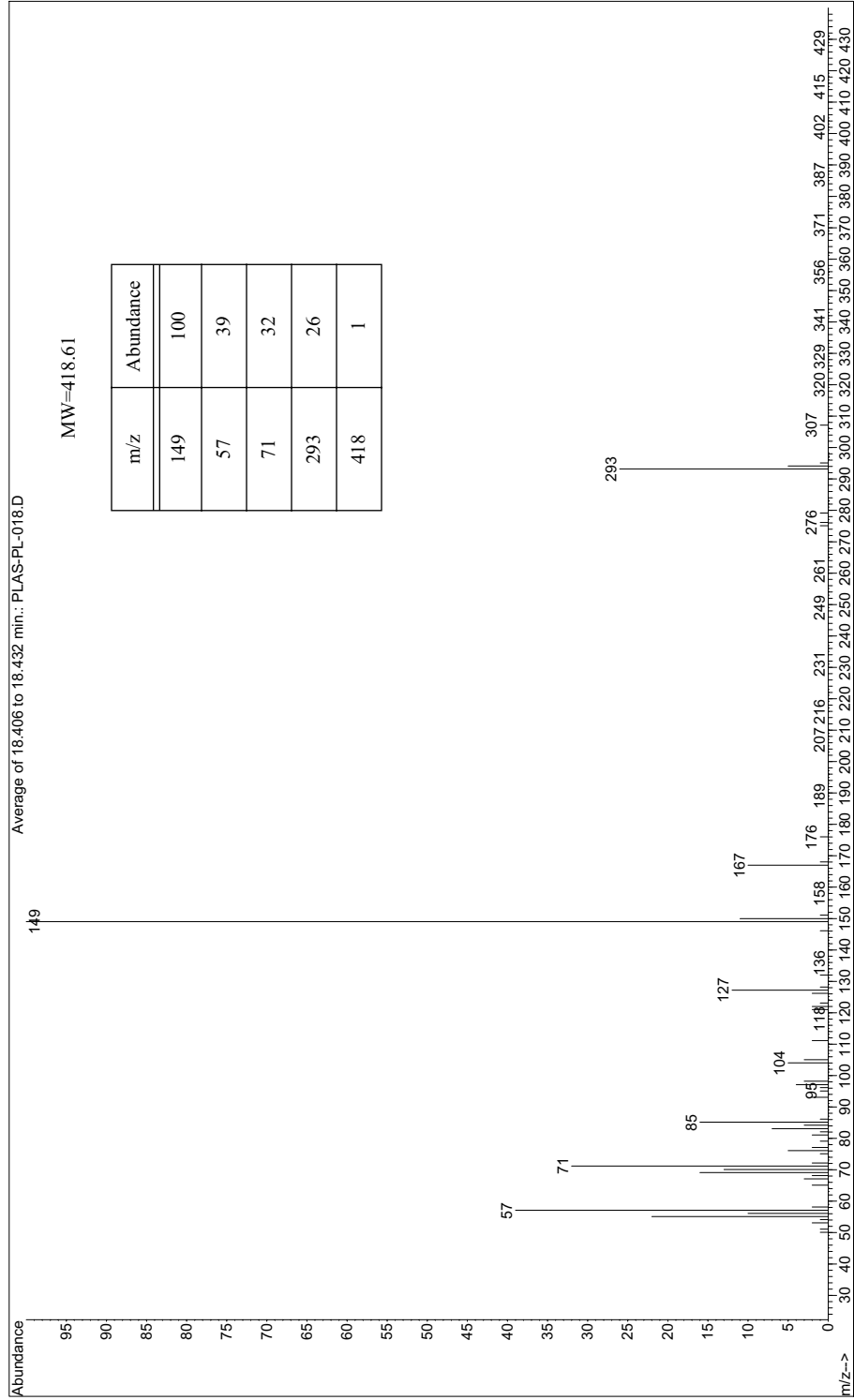
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Lowest published toxic oral dose (TDLo): 32900 mg/kg/70D-C [Rat].

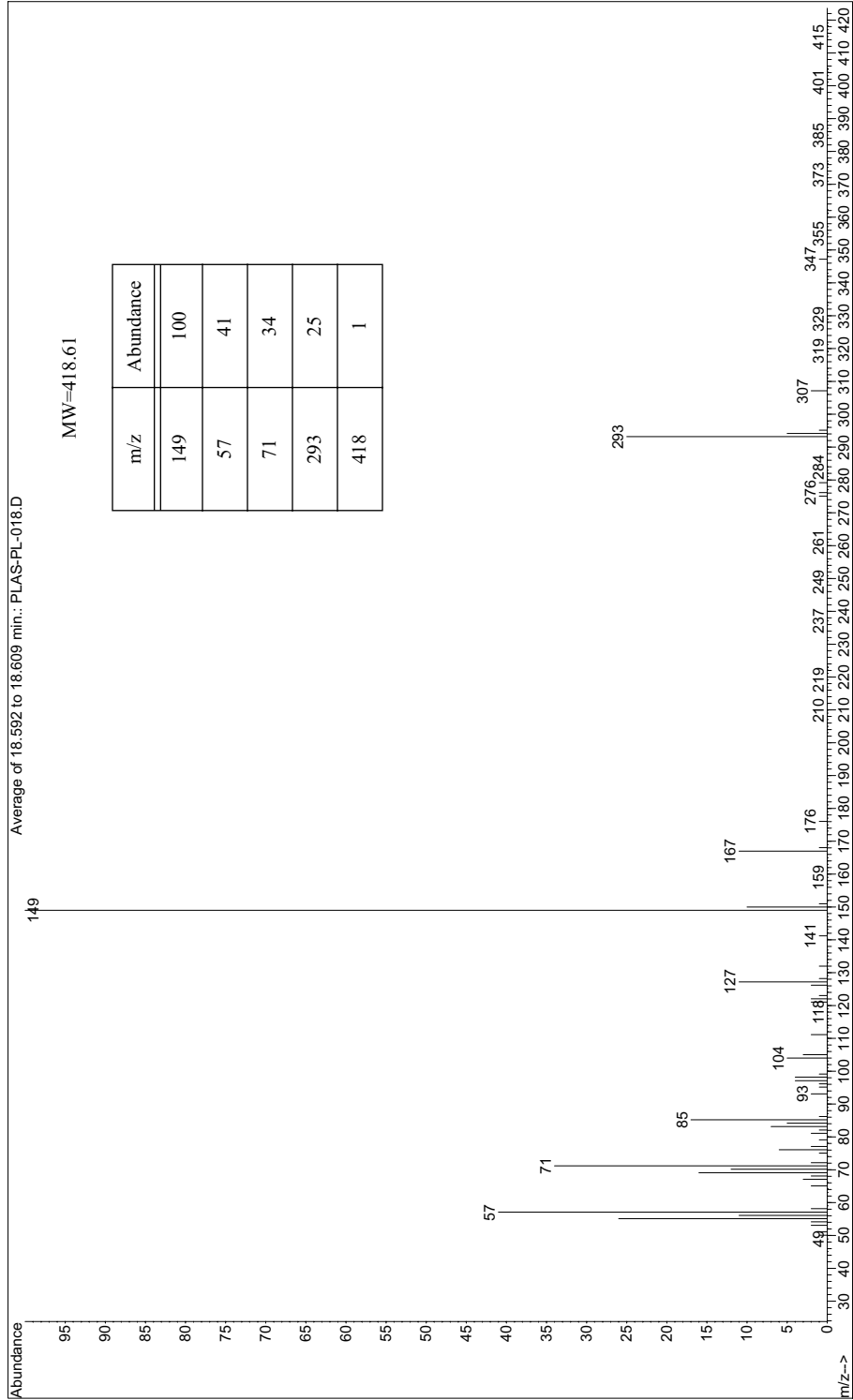
EPA lists as a suspected developmental toxin. Also produced kidney and liver effects when given to rodents in high oral doses.

Mass Spectrum for Jayflex® DINP - PLAS-PL-018



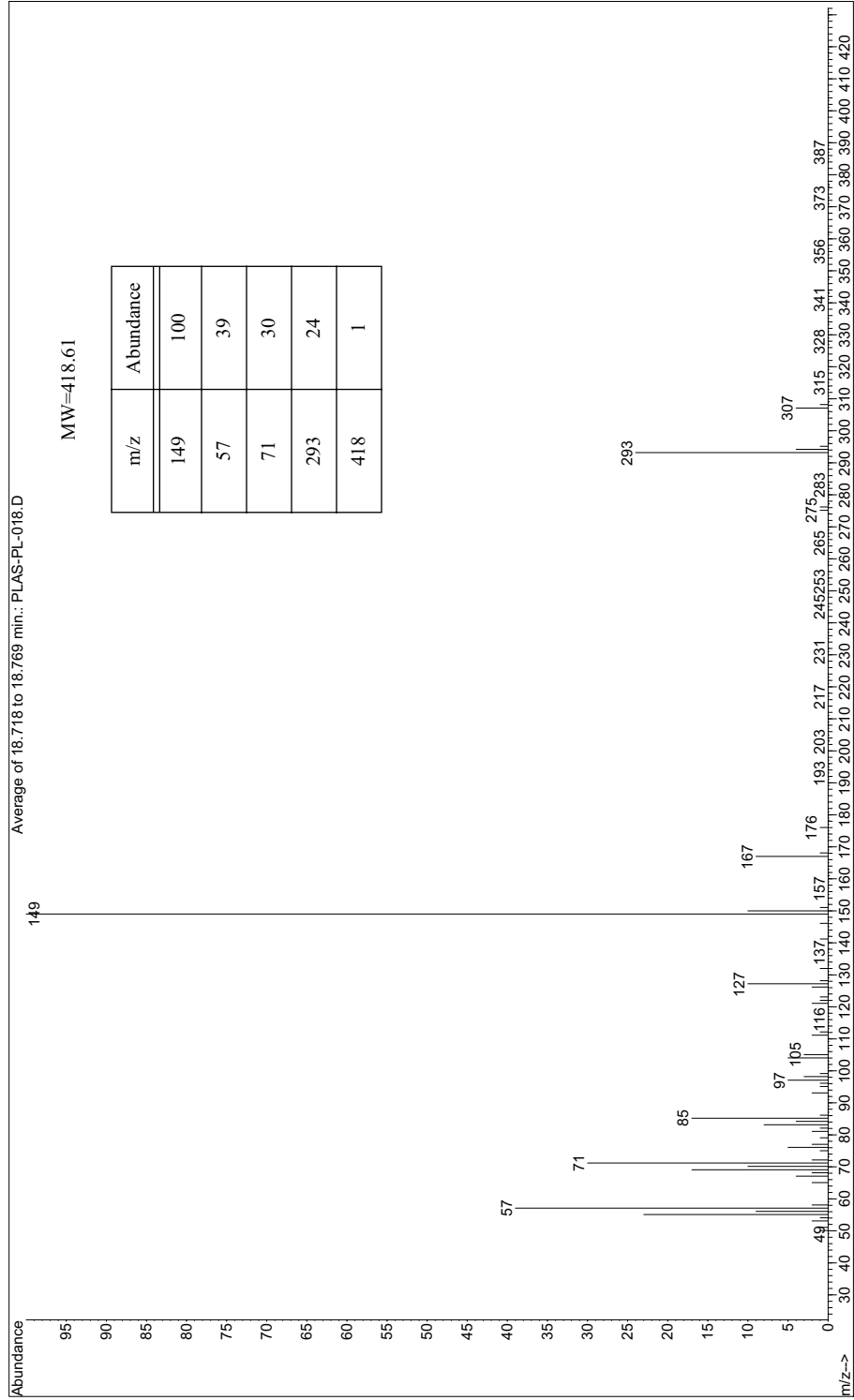
For Chromatogram See Appendix A - PLAS-PL-018 - page 573

Mass Spectrum for Jayflex® DINP - PLAS-PL-018



For Chromatogram See Appendix A - PLAS-PL-018 - page 573

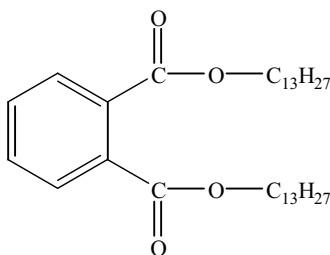
Mass Spectrum for Jayflex® DINP - PLAS-PL-018



For Chromatogram See Appendix A - PLAS-PL-018 - page 573

Jayflex® DTDP

ExxonMobil Corporation

**CAS Number** 68515-47-9**RTECS Number** N/A**Abbreviation** DTDP**Formula** C₃₄H₅₈O₄**Molecular Weight** 530.92**Chemical Name**

ditridecyl phthalate

Synonyms

1,2 benzenedicarboxylic acid, di-C11-14 branched alkyl ester

Brand Names & Manufacturers

Palatinol® 79P

BASF

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** Not available**Boiling Point** > 250 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	10-40	10-40	10-40	10-40	10-40

Application, Regulatory & Environmental Information

Application Highest molecular weight and most permanent monomeric phthalate plasticizer commercially available. Used for high temperature rated PVC insulation. Other end uses include traffic cones, automotive sealants, fabric coatings, fishing lures, and shoe compounds.

Regulatory Information

Does not have FDA approval for food contact applications.

Environmental Impact

This material is expected to be inherently biodegradable and has a low potential to bioaccumulate. It is not expected to be harmful to aquatic organisms. If released into the environment, it would be expected to partition to sediment and wastewater solids.

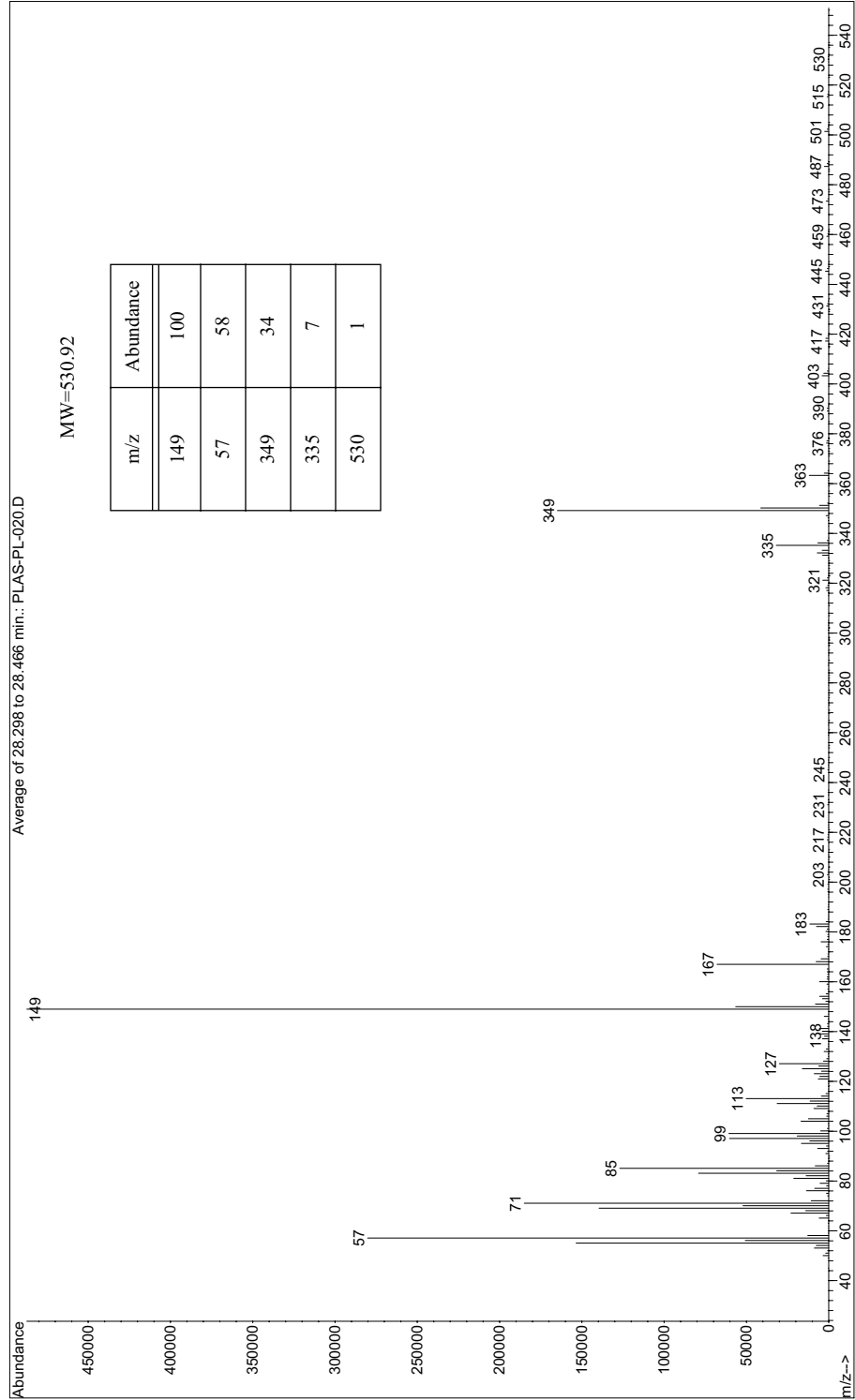
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

There are concerns regarding potential adverse health effects due to exposure to phthalates, particularly reproductive and developmental health effects.

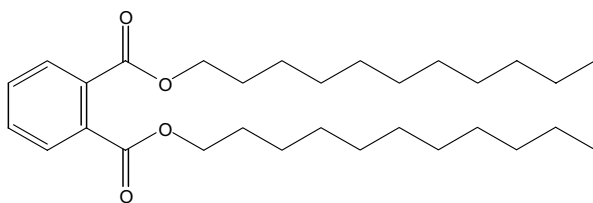
Mass Spectrum for Jayflex® DTDP - PLAS-PL-020



For Chromatogram See Appendix A - PLAS-PL-020 - page 574

Jayflex® L11P-E

ExxonMobil Corporation

**CAS Number** 3648-20-2**RTECS Number** TI1980000**Abbreviation** DUP**Formula** C₃₀H₅₀O₄**Molecular Weight** 474.72**Chemical Name**

diundecyl phthalate

Synonyms

DUP; 1,2-benzenedicarboxylic acid, diundecyl ester; phthalic acid, diundecyl ester

Brand Names & Manufacturers

Palatinol® 11P-I

BASF

Santicizer® 711

Solutia Inc.

Physical Properties**Appearance** Clear liquid with a characteristic odor**Melting Point** Not available**Boiling Point** 523 °C**Stability** Stable under normal conditions of use.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.1	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Highly permanent, low volatility, linear plasticizer used in wire and cable insulation for automotive and communications applications, low temperature, high performance film and sheeting as well as low fogging automotive interiors.

Regulatory Information

Diundecyl phthalate is FDA approved for use as a component of poly (p-methylstyrene) and rubber-modified poly (p-methylstyrene) intended for use in contact with food, subject to 21CFR177.1635.

Environmental Impact

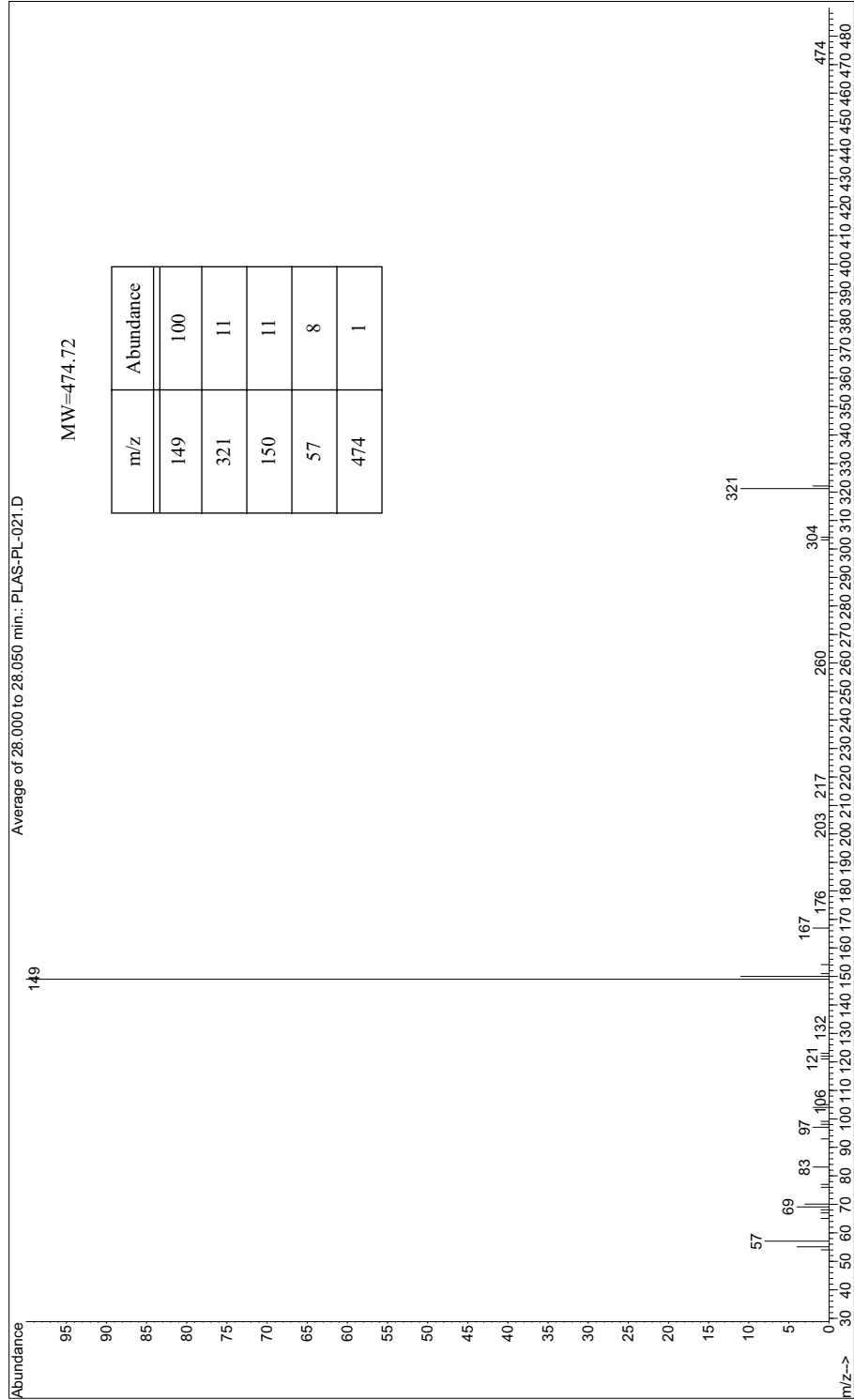
This material is expected to be inherently biodegradable and has a low potential to bioaccumulate. It is not expected to be harmful to aquatic organisms. If released into the environment, it would be expected to partition to sediment and wastewater solids.

Point of Release

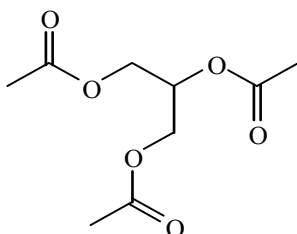
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological DataNot listed by ACGIH, IARC, NTP, or OSHA as a cancer causing agent. Acute intraperitoneal LD50 >15.8 g/kg [Mouse]; acute dermal (LD50): >10 g/kg [Rabbit]; acute oral (LD50): >20 g/kg [Rat]; acute inhalation (LC50 6 hour) >6040 mg/m³ [Rat].

Mass Spectrum for Jayflex® L11P-E - PLAS-PL-021



For Chromatogram See Appendix A - PLAS-PL-021 - page 575

Kesscoflex TRA**CAS Number** 102-76-1**RTECS Number** AK3675000**Abbreviation** Not Identified**Formula** C₉H₁₄O₆**Molecular Weight** 218.20**Chemical Name**

1,2,3-propanetriol triacetate

Synonyms

triacetin; glycerol triacetate; glyceryl triacetate

Brand Names & ManufacturersKodaflex[®] triacetin

Eastman Chemical

Physical Properties**Appearance** Colorless, oily liquid**Melting Point** 3 °C**Boiling Point** 259 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	70	40-80	40-80	U	U	U

Application, Regulatory & Environmental Information

Application Plasticizer for cellulose nitrate (commonly used in cigarette filters). Also used as a solvent for basic dyes, fixative in perfumery, food additive, pharmaceuticals, and photographic films.

Regulatory Information

Triacetin is approved by the FDA for direct and indirect food contact applications.

Environmental Impact

Triacetin is readily biodegradable. The chemical is expected to have a low potential for bioaccumulation based on a low log Pow (0.21). Considered to be nontoxic to aquatic organisms and birds.

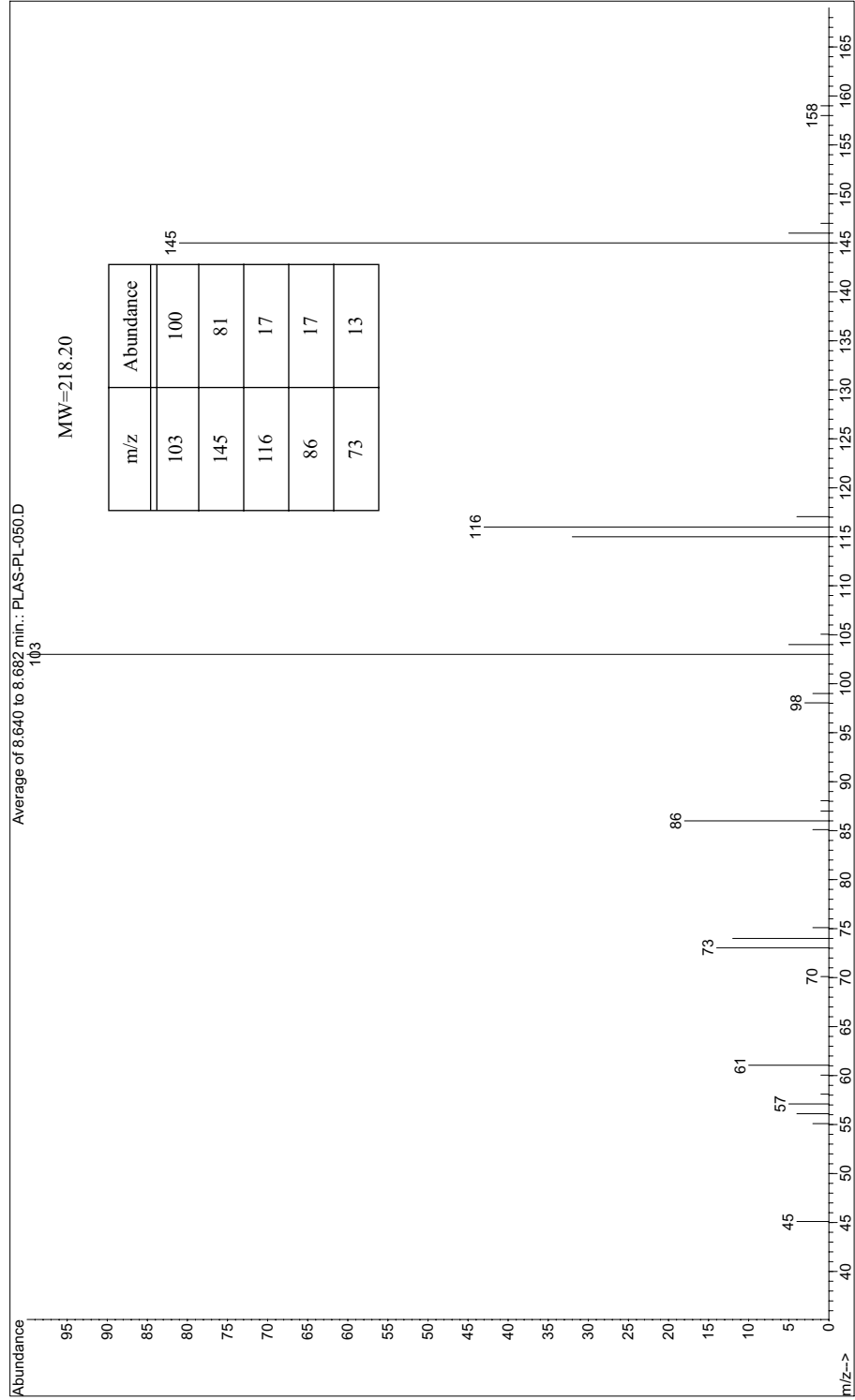
Point of Release

Environmental exposure may occur from emission to aquatic compartment from wastewater and evaporative emissions associated with its use in the perfume and cosmetic industries and its use as a solvent and CO₂ remover from natural gas, and disposal of consumer products containing triacetin.

Toxicological Data

Based on the available data and anticipated daily intake (7.8 mg/day/adult), triacetin and a group of related triglycerides did not represent a hazard to human health.

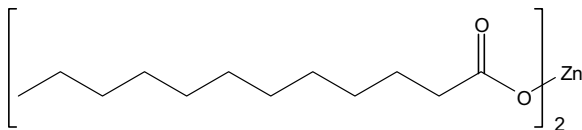
Mass Spectrum for Kesscoflex TRA - PLAS-PL-050



For Chromatogram See Appendix A - PLAS-PL-050 - page 576

Laurex[®]

Chemtura Corporation



CAS Number N/A

RTECS Number N/A

Abbreviation Not Identified

Formula C₂₄H₄₆O₄Zn

Molecular Weight 464.01

Chemical Name

zinc salt of lauric and related fatty acids

Synonyms

N/A

Brand Names & Manufacturers

Laurex

Chemtura Corporation

Physical Properties**Appearance** Tan, flaked solid**Melting Point** 107-118 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone <0.1	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application** Activator and plasticizer for general use in natural and synthetic rubber products.**Regulatory Information**

FDA approved by 21CFR175.105 — Adhesives — No Limitations and 177.2600 — Rubber Articles Intended for Repeated Use — 5% Max.

Environmental Impact

This compound is the zinc salt of a mixture of fatty acids, predominantly lauric acid, which is one of the three most widely distributed saturated fatty acids found in nature (coconut and palm oils). Consequently, no hazardous environmental impact is expected.

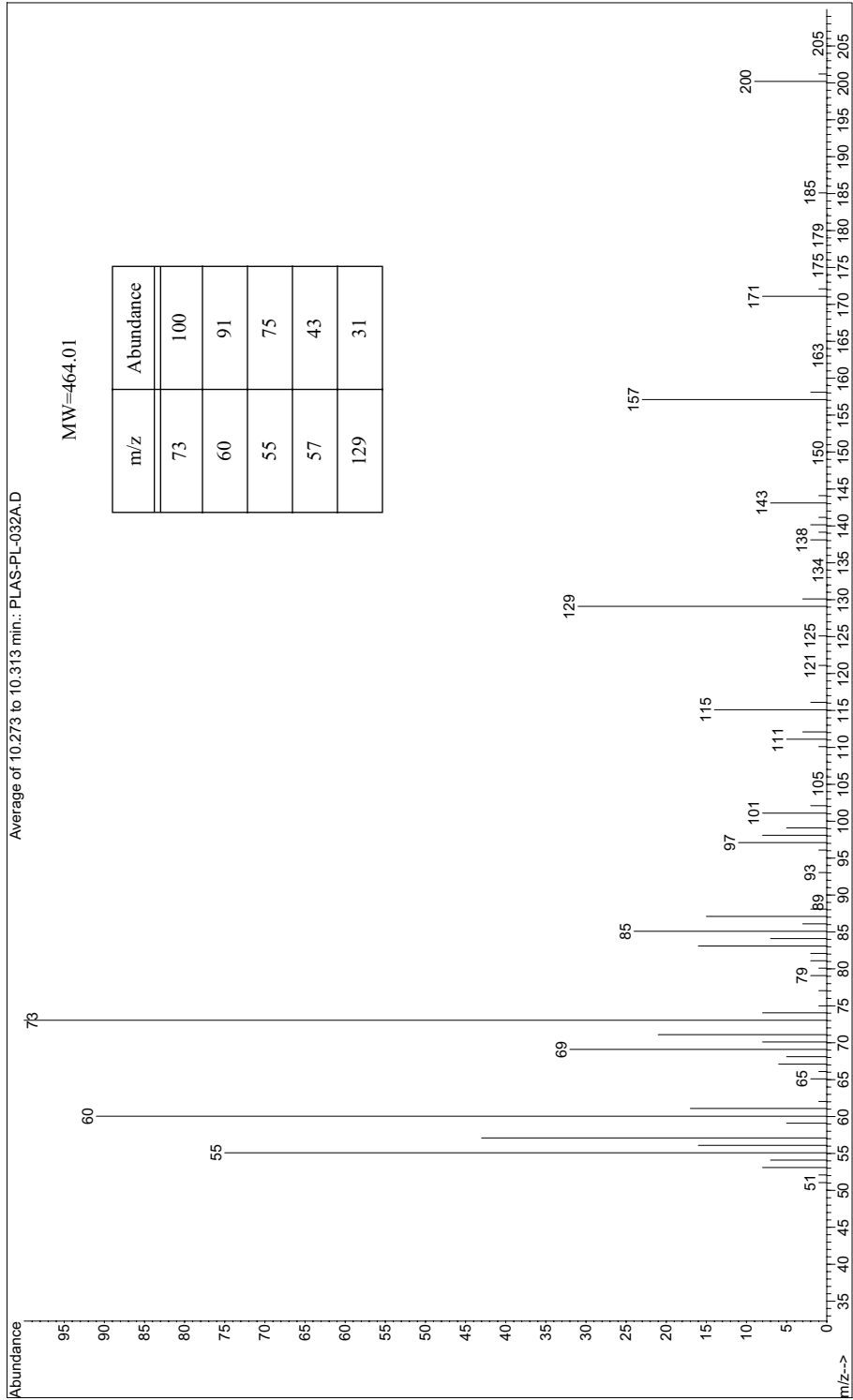
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

No health hazards have been identified.

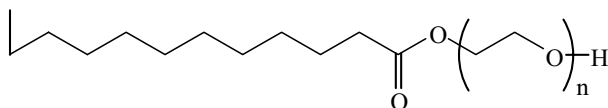
Mass Spectrum for Laurex® - PLAS-PL-032



For Chromatogram See Appendix A - PLAS-PL-032 - page 577

Markstat® 51

Chemtura Corporation

**CAS Number** 9004-81-3**RTECS Number** TQ8701000**Abbreviation** Not Identified**Formula** $(C_2H_4O)_n C_{12}H_{24}O_2$ **Molecular Weight** ~400**Chemical Name**

poly(ethylene glycol) monolaurate

Synonyms

polyethylene glycol laurate; polyglycolester; polyoxyethylene monolaurate

Brand Names & Manufacturers

Markstat 51

Chemtura Corporation

Physical Properties**Appearance** Clear, yellowish, medium viscosity liquid**Melting Point** Not available**Boiling Point** 260 °C**Stability** Stable, however discoloration may occur on exposure to air.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	E	U	U	U	U	<0.1

Application, Regulatory & Environmental Information**Application** Antistatic plasticizer used for PVC flooring, conveyor belts, hoses, and plastic film.**Regulatory Information**

Has FDA approval under Section 178.3910 to be used in surface lubricants for rolling of metallic foil or sheet stock provided that total residual lubricant remaining on the metallic article in the form in which it contacts food does not exceed 0.015 mg per square inch of metallic food-contact surface.

Environmental Impact

This material is expected to be inherently biodegradable and has a low potential to bioaccumulate. It is not expected to be harmful to aquatic organisms.

Point of Release

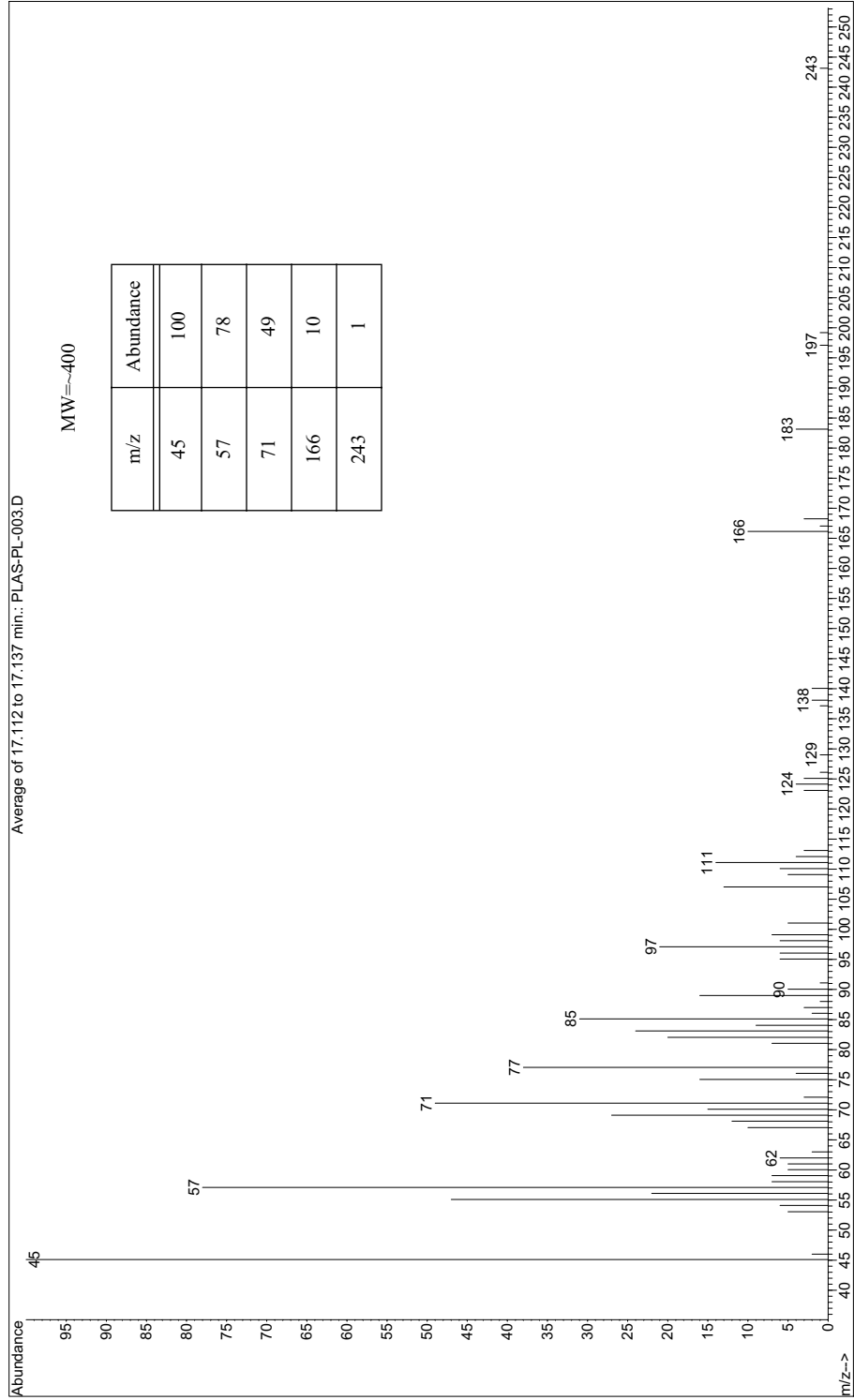
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

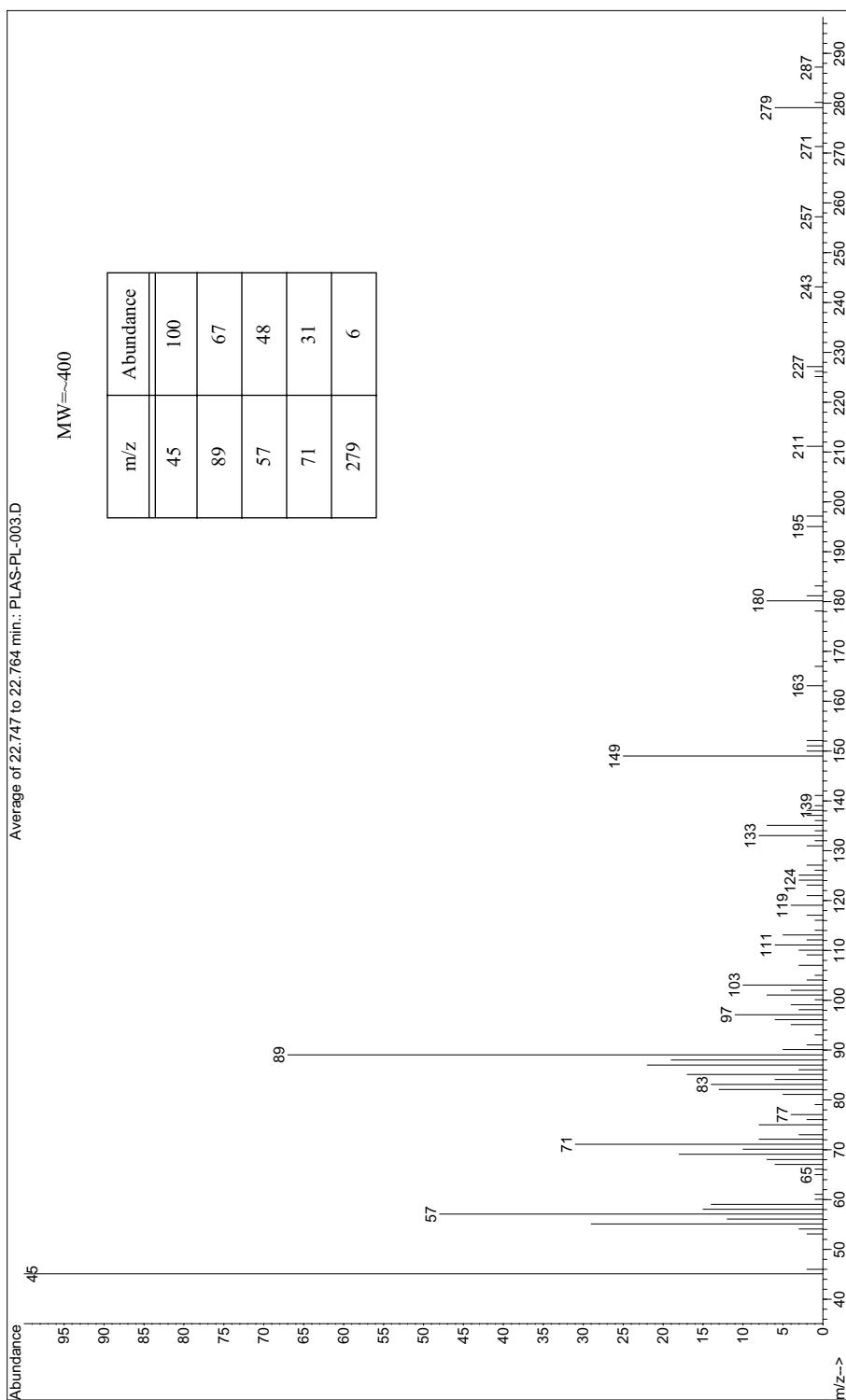
Acute oral toxicity (LD50): >2500 mg/kg [Mouse].

Lowest published toxic dose (TDLo): 889 gm/kg/70D-C [Rat].

Mass Spectrum for Markstar® 51 - PLAS-PL-003

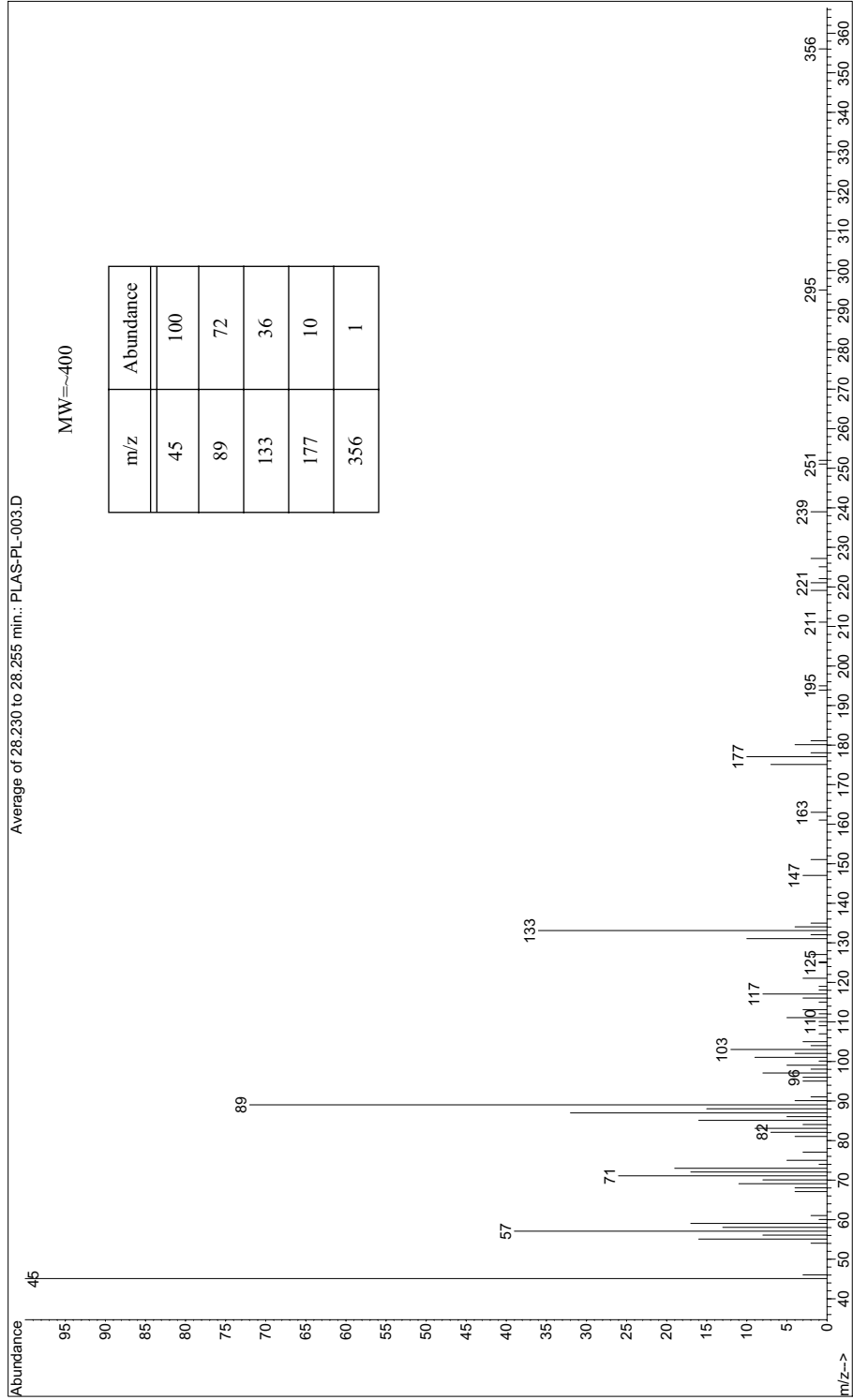


For Chromatogram See Appendix A - PLAS-PL-003 - page 578

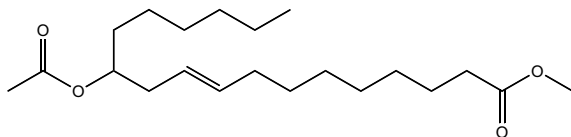
Mass Spectrum for Markstat® 51 - PLAS-PL-003

For Chromatogram See Appendix A - PLAS-PL-003 - page 578

Mass Spectrum for Markstar® 51 - PLAS-PL-003



For Chromatogram See Appendix A - PLAS-PL-003 - page 578

Methyl O-Acetylricinoleate**CAS Number** 140-03-4**RTECS Number** VJ3410000**Abbreviation** MAR**Formula** C₂₁H₃₈O₄**Molecular Weight** 354.52**Chemical Name**

methyl (Z)-12-acetyloxyoctadec-9-enoate

Synonyms

methyl (Z)-12-acetyloxyoctadec-9-enoate; 12-(acetyloxy)-9-octadecenoic acid, methyl ester

Brand Names & Manufacturers

Flexricin® P4

Vertellus

Naturechem MAR

HallStar

Physical Properties**Appearance** Pale yellow liquid**Melting Point** -26°C**Boiling Point** 185°C**Stability** Stable under normal conditions of use.**Solubility**
(g/100mL 20°C)**Water**
U**MeOH**
S**EtOH**
S**Acetone**
U**CH₂Cl₂**
U**Hexane**
U**Application, Regulatory & Environmental Information****Application**

All-purpose plasticizer for lacquers and vinyls. It is a plasticizer and processing aid for rubber compounds. It is a low volatility, low viscosity product which imparts exceptional cold crack resistance to flexible nitrocellulose lacquers.

Regulatory Information

Not intended for use in applications that come in contact with food or in products which may come in contact with mucous membranes or abraded skin or be implanted into the body.

Environmental Impact

An estimated log Kow of 7.48 suggests the potential for significant bioaccumulation.

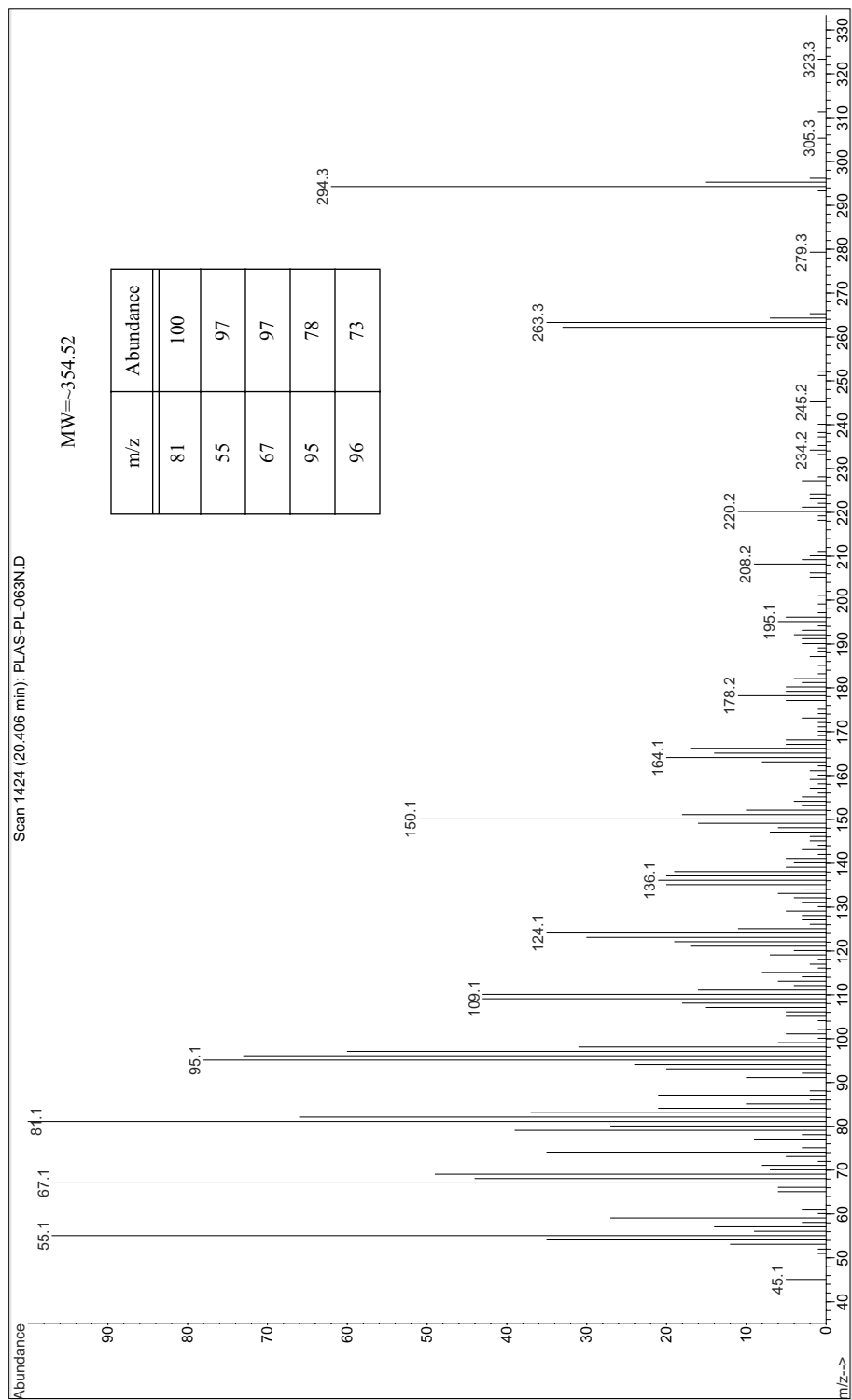
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral LD50: > 4800 mg/kg [Rat].

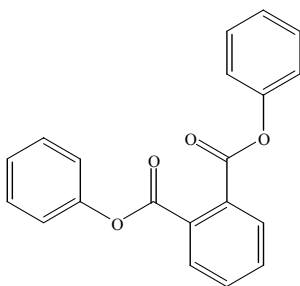
Mass Spectrum for Methyl O-Acetylricinoleate - PLAS-PL-063



For Chromatogram See Appendix A - PLAS-PL-063 - page 579

Morflex® 150

Morflex, Inc.

**CAS Number** 84-61-7**RTECS Number** TI0889000**Abbreviation** DCHP**Formula** C₂₀H₂₆O₄**Molecular Weight** 330.46**Chemical Name**

dicyclohexyl phthalate

Synonyms

phthalic acid, dicyclohexyl ester; 1,2-benzenedicarboxylic acid, dicyclohexyl ester

Brand Names & Manufacturers

Unimoll® 66

Lanxess Corp

Physical Properties**Appearance** White powder**Melting Point** 63 °C**Boiling Point** 200-235 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application** Used as a plasticizer in heat-sealable films, adhesives, coatings, under floor sealing compounds, and as a co-plasticizer in PVC.**Regulatory Information**

This product does not have FDA approval for food contact applications.

Environmental Impact

Log Kow value of 5.6 indicates that this material is likely to bioaccumulate. It is not readily biodegradable and considered to be toxic to aquatic organisms.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

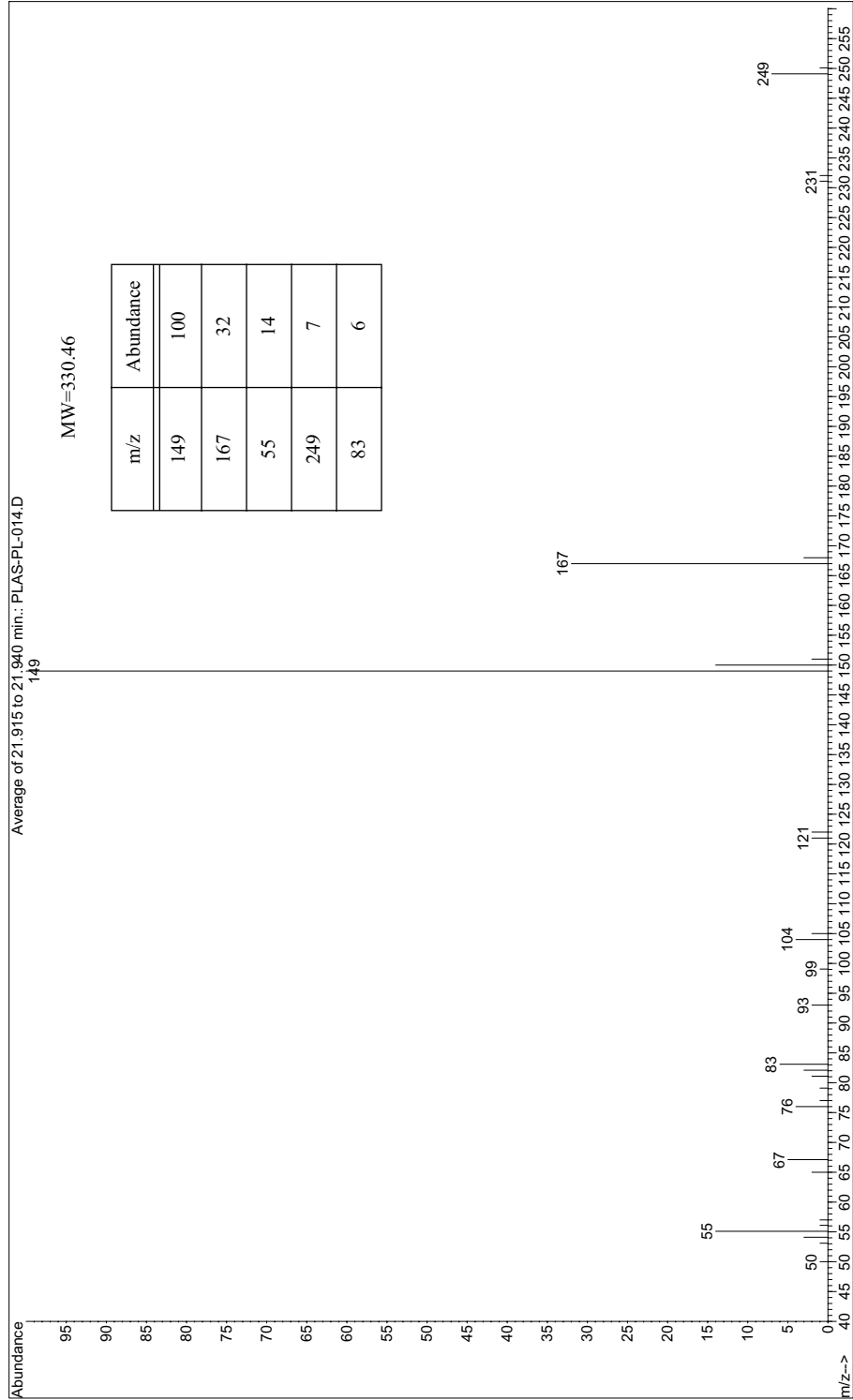
Toxicological Data

Acute oral toxicity (LD50): 30 mL/kg [Rat]

Lowest published toxic oral dose (TDL_o): 10500 mg/kg/7D-C [Rat].

Suspected endocrine toxicant.

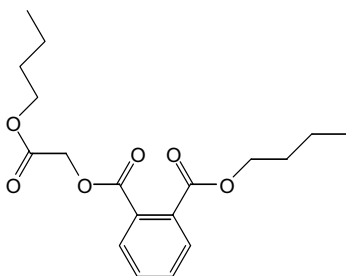
Mass Spectrum for Morflex® 150 - PLAS-PL-014



For Chromatogram See Appendix A - PLAS-PL-014 - page 580

Morflex® 190

Morflex, Inc.

**CAS Number** 85-70-1**RTECS Number** TI 0535000**Abbreviation** Not Identified**Formula** C₁₈H₂₄O₆**Molecular Weight** 336.38**Chemical Name**

butylphthalyl butyl glycolate (with <10% dibutyl phthalate)

Synonyms

dibutyl O-(o-carboxybenzoyl) glycolate; butyl carbobutoxymethyl phthalate; butyl glycolyl butyl phthalate

Brand Names & Manufacturers

Santicizer® B-16

Solutia Inc.

Physical Properties**Appearance** Clear liquid**Melting Point** <25 °C**Boiling Point** 220 °C (10 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application** Used as a plasticizer in food-packaging material, PVC tubing, and dental cushions.**Regulatory Information**

Morflex® 190 is FDA approved for direct food contact. This product contains <10% dibutyl phthalate which is a SARA 313 reportable compound.

Environmental Impact

The primary component, butylphthalyl butyl glycolate (BPBG), is expected to rapidly hydrolyze in environmental media under aerobic conditions. The dibutyl phthalate (DBP) is also expected to hydrolyze in environmental media; however, the DBP may be toxic to some aquatic organisms.

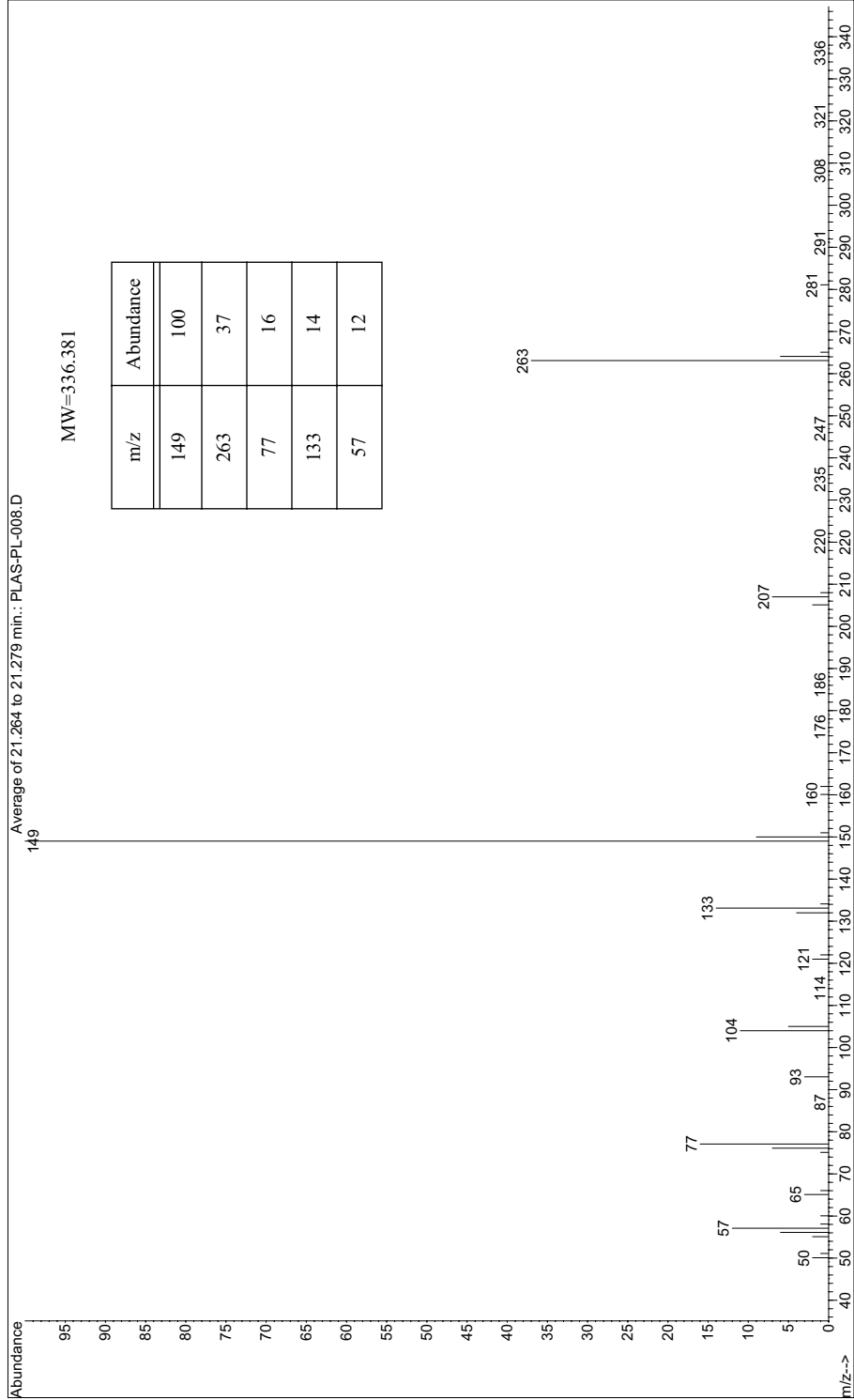
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

While neither component is classified as a carcinogen by IARC, NTP, or OSHA, repeated or prolonged exposure to dibutyl phthalate may lead to adverse health effects.

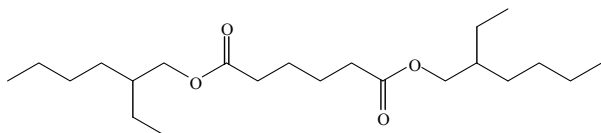
Mass Spectrum for Morflex® 190 - PLAS-PL-008



For Chromatogram See Appendix A - PLAS-PL-008 - page 581

Morflex® 310

Morflex, Inc.

**CAS Number** 103-23-1**RTECS Number** AU9700000**Abbreviation** DOA/DEHA**Formula** C₂₂H₄₂O₄**Molecular Weight** 370.57**Chemical Name**

hexanedioic acid, bis(2-ethylhexyl) ester; dioctyl adipate; di-(2-ethylhexyl) adipate; bis(2-ethylhexyl)hexanedioate

Synonyms

N/A

Brand Names & ManufacturersPlasthall® DOA
Santicizer® DOAHallStar
Solutia Inc.**Physical Properties****Appearance** Colorless, oily liquid with an aromatic odor**Melting Point** -67.8 °C**Boiling Point** 417 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	U	40-80	U	U

Application, Regulatory & Environmental Information**Application** DEHA is a plasticizer used primarily in food-contact wrapping, building materials, and household furnishings.**Regulatory Information**

Monitored under the federal Safe Drinking Water Act due to potential adverse health effects. It is approved by the FDA for food contact applications.

Environmental Impact

This substance is harmful to aquatic organisms and has a low bioaccumulation potential. It is readily degradable via abiotic (hydrolysis) and biotic processes.

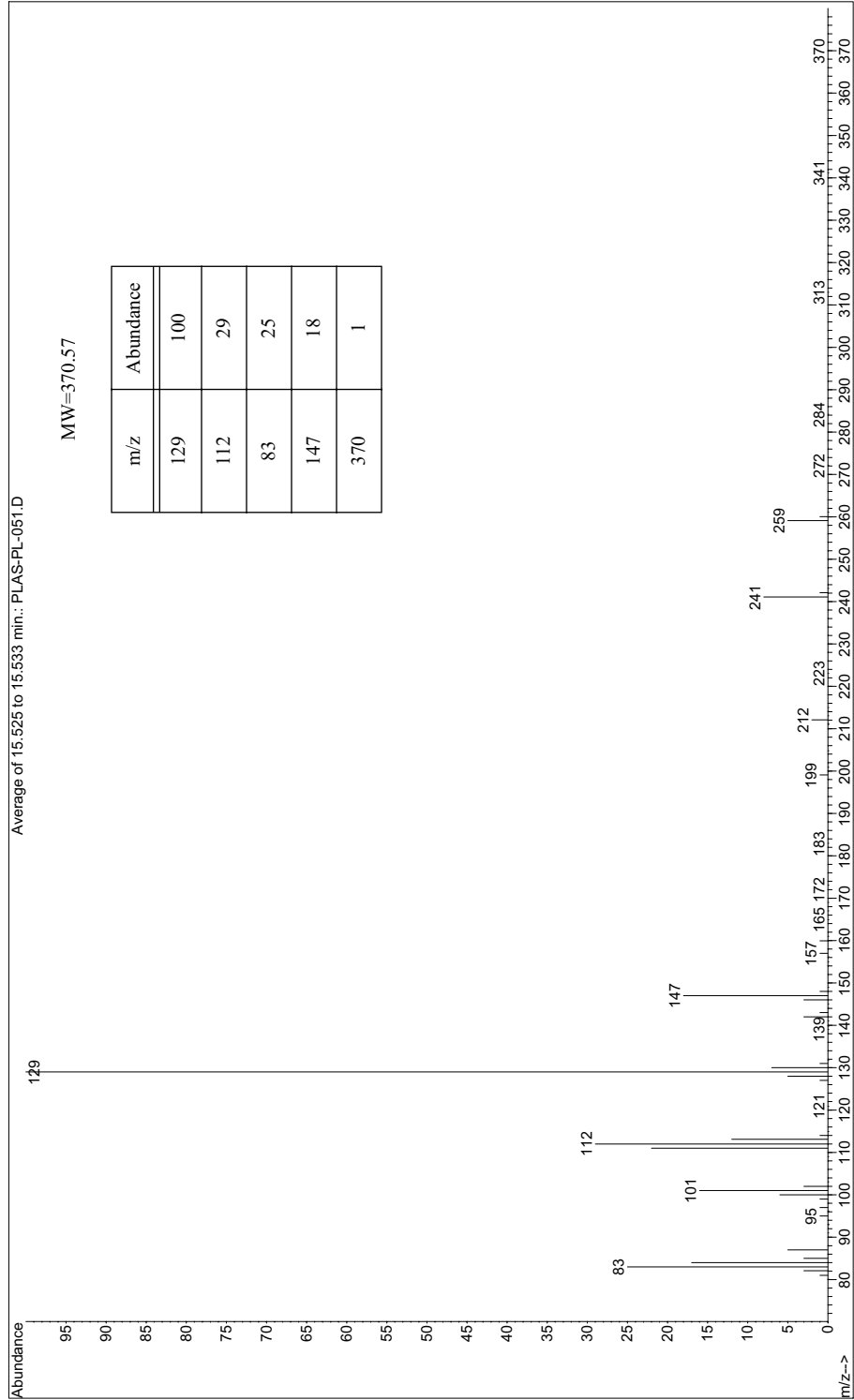
Point of Release

Occupational exposures are low based on production in a closed system and its low vapor pressure. The estimated exposure levels to the general population via consumer products, migration of DEHA from food wraps, is estimated at exposures of 117 µg/kg/d. The highest measured surface water concentration was 0.001 mg/L. Both of these results are considered to be low as well.

Toxicological Data

This product is a suspected carcinogen and endocrine toxicant. Classified as a possible developmental toxin. This substance is toxic to blood, the reproductive system, liver, and upper respiratory tract.

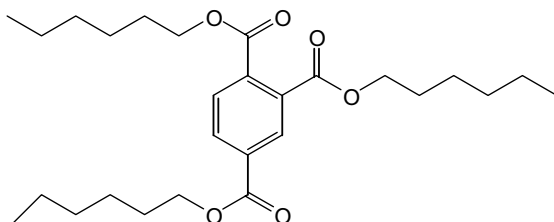
Mass Spectrum for Morflex® 310 - PLAS-PL-051



For Chromatogram See Appendix A - PLAS-PL-051 - page 582

Morflex® 560

Morflex, Inc.

**CAS Number** 1528-49-0**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₇H₄₂O₆**Molecular Weight** 462.62**Chemical Name**

tri-n-hexyl trimellitate

Synonyms

trihexyl benzene-1,2,4-tricarboxylate

Brand Names & Manufacturers

Morflex 560

Morflex, Inc.

Physical Properties**Appearance** Oily liquid**Melting Point** -45.5 °C**Boiling Point** 260 - 262 °C (4 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-50

Application, Regulatory & Environmental Information

Application Primarily used as a plasticizer for PVC and its copolymers. Vinyls plasticized with this ester find application in variety of markets including automotive and furniture upholstery, wire coatings, and gasketing materials.

Regulatory Information

This product does not have FDA approval for direct or indirect food contact. It is not considered to be hazardous for shipping purposes.

Environmental Impact

The environmental fate of this product has not been thoroughly investigated.

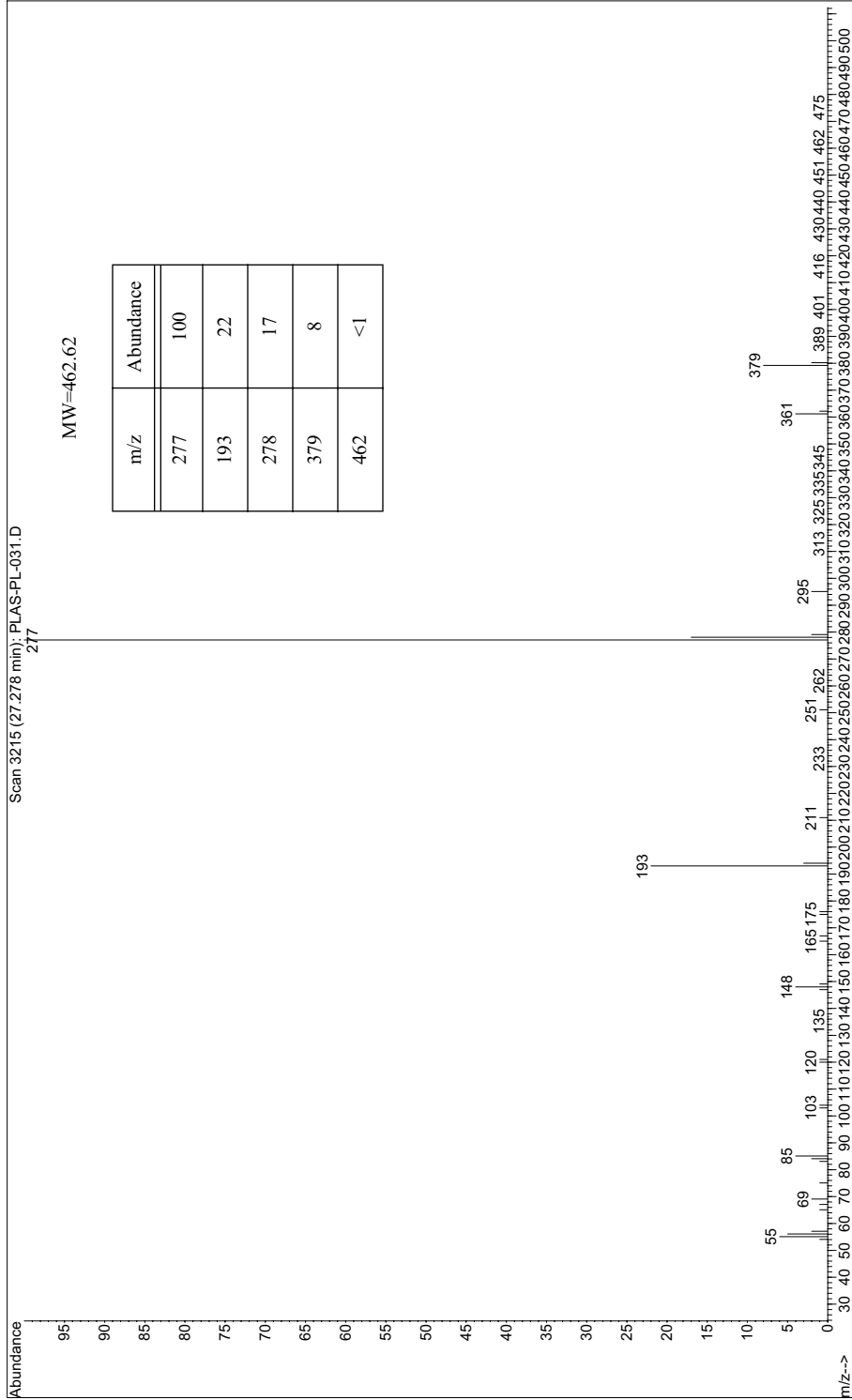
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

This product is not classified as a carcinogen by IARC, NTP, or OSHA and the potential human health effects due to exposure are unknown.

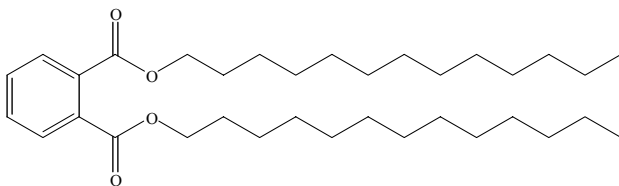
Mass Spectrum for Morflex® 560 - PLAS-PL-031



For Chromatogram See Appendix A - PLAS-PL-031 - page 583

Morflex® x-1125

Morflex, Inc.

**CAS Number** 119-06-2**RTECS Number** TI1950000**Abbreviation** DTDP**Formula** C₃₄H₅₈O₄**Molecular Weight** 530.93**Chemical Name**

1,2-benzenedicarboxylic acid, ditridecyl ester

Synonyms

di(tridecyl) phthalate; phthalic acid, ditridecyl ester

Brand Names & Manufacturers

Jayflex® DTDP

Exxon Mobil Chemical

Physical Properties**Appearance** Clear, viscous liquid**Melting Point** Not available**Boiling Point** >285 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	10-40	10-40	10-40	10-40	10-40

Application, Regulatory & Environmental Information**Application** High temperature PVC insulation for wire and cable.**Regulatory Information**

This material does not have FDA approval for food contact applications.

Environmental Impact

Phthalates are now being detected routinely in a range of environmental water samples including drinking water. They are widely dispersed in the environment. Due to the poor solubility of phthalates, sediments are the ultimate sink for phthalates released into the aquatic environment. Phthalates can accumulate in environments that are highly anaerobic and poorly colonized by microbes. Furthermore, cold environmental conditions slow their biodegradation.

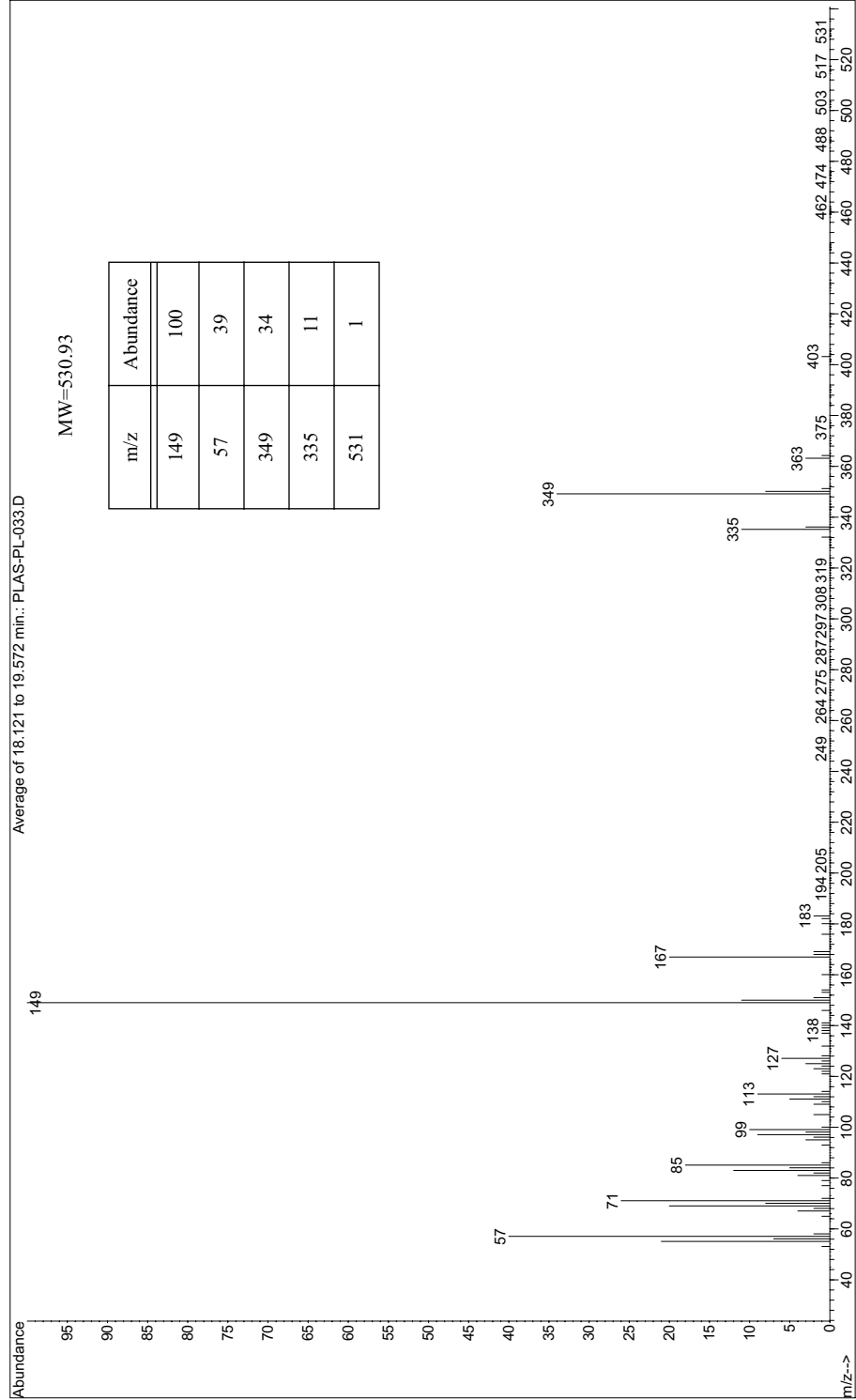
Point of Release

Can be released as point source pollution during production, distribution, and incorporation into PVC resin. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Suspected endocrine toxin. (LD50): >2000 mg/kg [Rat].

Mass Spectrum for Morflex® x-1125 - PLAS-PL-033



For Chromatogram See Appendix A - PLAS-PL-033 - page 584

Paraplex® G-30

HallStar

Unspecified Structure

CAS Number N/A

RTECS Number N/A

Abbreviation Not Identified

Formula N/A

Molecular Weight ~800

Chemical Name

proprietary dibasic acid polyester mixture

Synonyms

N/A

Brand Names & Manufacturers

Paraplex G-30

HallStar

Physical Properties
Appearance Light yellow, viscous liquid; slight ester odor**Melting Point** Not available**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	U	U	U

Application, Regulatory & Environmental Information
Application Low molecular weight polymeric plasticizer used in electrical wire insulation and coatings for wood, metal, fabrics, and paper.**Regulatory Information**

Does not have FDA approval for food contact and is not regulated as a hazardous waste by the EPA.

Environmental Impact

The 48-hour EC50 is 14 mg/L. The 48-hour NOEC is 5.2 mg/L.

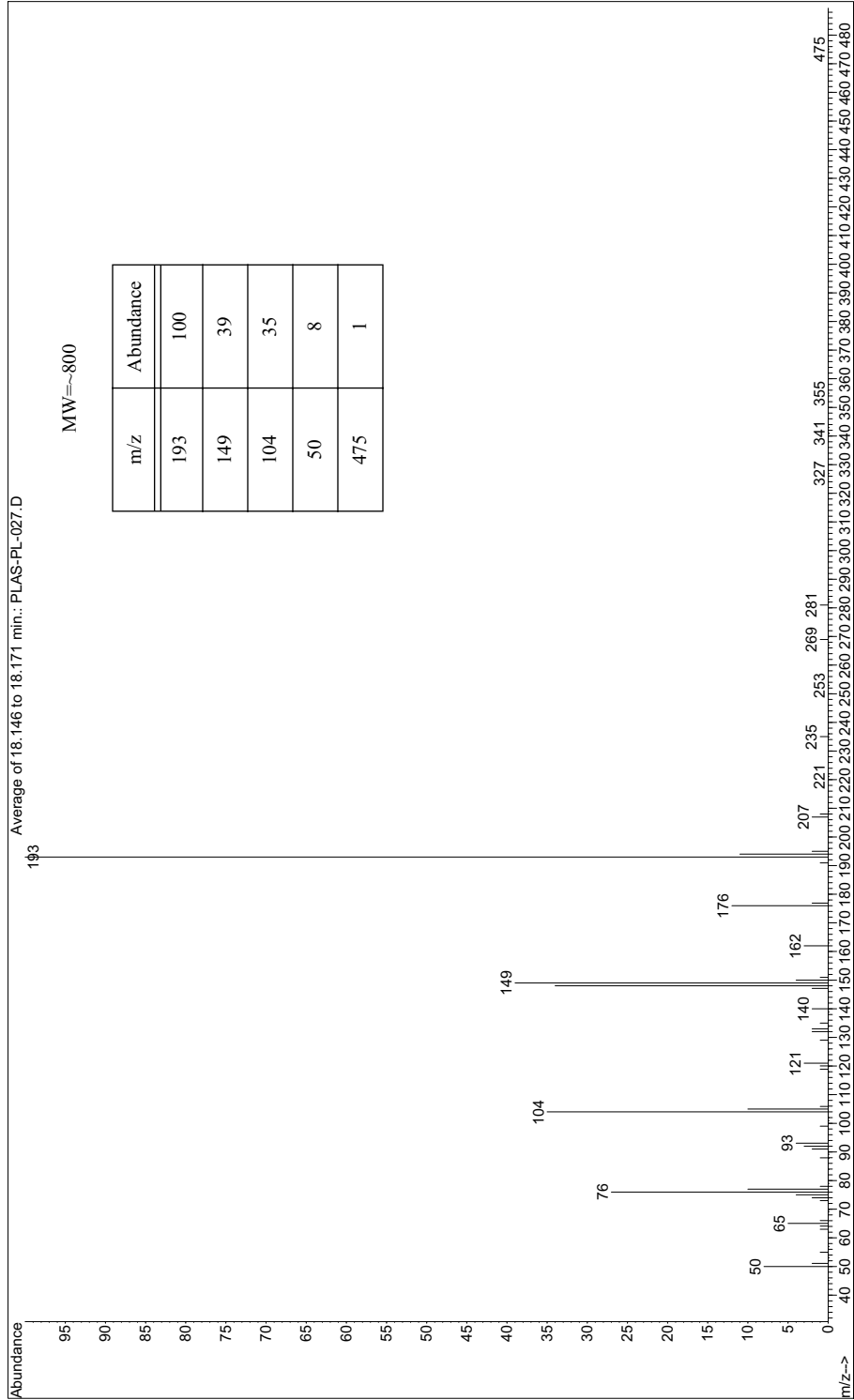
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

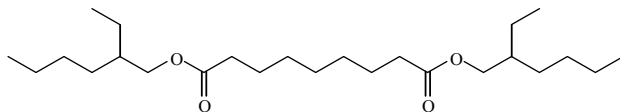
Toxicological Data

Oral (LD50): > 5.0 g/kg [Rat]. Primary dermal irritation: 1.0 (PII). No evidence of corrosion was noted. Not a primary irritant. Primary ocular irritation: No evidence of corrosion was noted.

Mass Spectrum for Paraplex® G-30 - PLAS-PL-027



For Chromatogram See Appendix A - PLAS-PL-027 - page 585

Plasthall® DOZ

CAS Number 2064-80-4
RTECS Number CM2000000
Abbreviation DOZ

Formula C₂₅H₄₈O₄
Molecular Weight 412.65

Chemical Name

nonanedioic acid, dioctyl ester

Synonyms

dioctyl azelate; azelaic acid, dioctyl ester

Brand Names & Manufacturers

Kodaflex® DOZ Eastman Chemical
 Novaflex® DOZ Cross Tech

Physical Properties**Appearance** Clear liquid**Melting Point** Not available**Boiling Point** 376 °C**Stability**

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	1-10	40-80	40-80	U	U	U

Application, Regulatory & Environmental Information

Application Used in conjunction with a monomeric plasticizer and a metal oxide to make an inherently hydrophobic material more hydrophilic. Commonly used in toys and medical equipment.

Regulatory Information

FDA approved in polymeric substances and as a component of adhesives intended for use in contact with food.

Environmental Impact

Listed as a moderate health priority based on persistence and bioaccumulative studies as of July 2006.

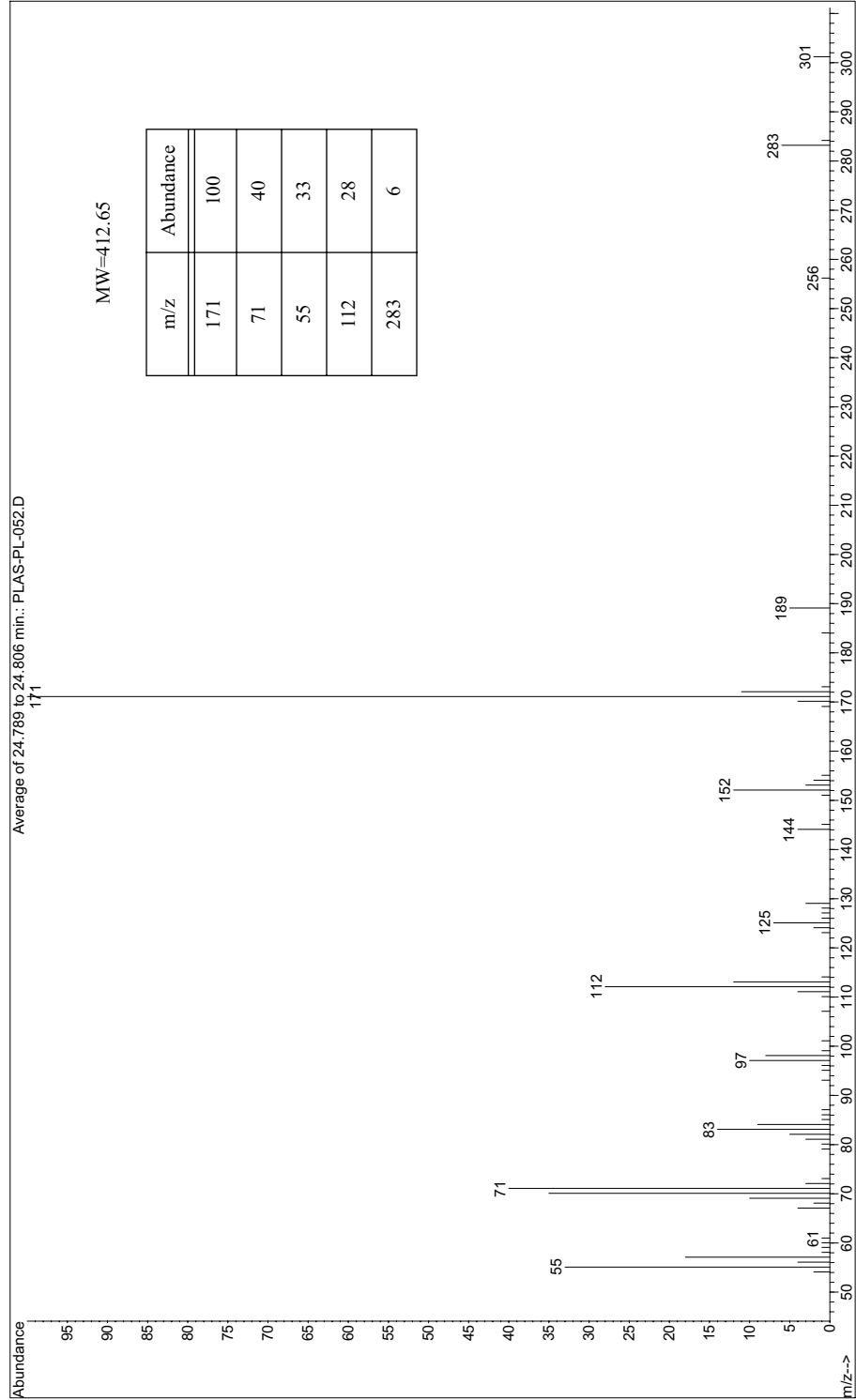
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

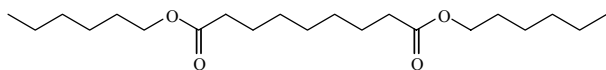
Mass Spectrum for Plasthall® DOZ - PLAS-PL-052



For Chromatogram See Appendix A - PLAS-PL-052 - page 586

Plastolein 9050

Cognis Corporation

**CAS Number** 109-31-9**RTECS Number** CM2100000**Abbreviation** DnHA**Formula** C₂₁H₄₀O₄**Molecular Weight** 356.54**Chemical Name**

nonanedioic acid, dihexyl ester

Synonyms

dihexyl azelate; azelaic acid, dihexyl ester

Brand Names & Manufacturers

Plastolein 9050

Cognis Corporation

Physical Properties**Appearance** Colorless liquid**Melting Point** -80.0 °C**Boiling Point** 282 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.	40-80	40-80	U	U	U

Application, Regulatory & Environmental Information

Application Used as a plasticizer in the production of polyvinyl chloride, polystyrene, and other plastics used for food, drinks, and polypropylene food wrap.

Regulatory Information

FDA approved for use as a plasticizer at levels not exceeding 24% by weight of the permitted plastic substance used in contact with non-fatty foods and non-alcoholic beverages or fatty foods containing less than 30% fat or oil content.

Environmental Impact

Long-term environmental impact studies have not been completed.

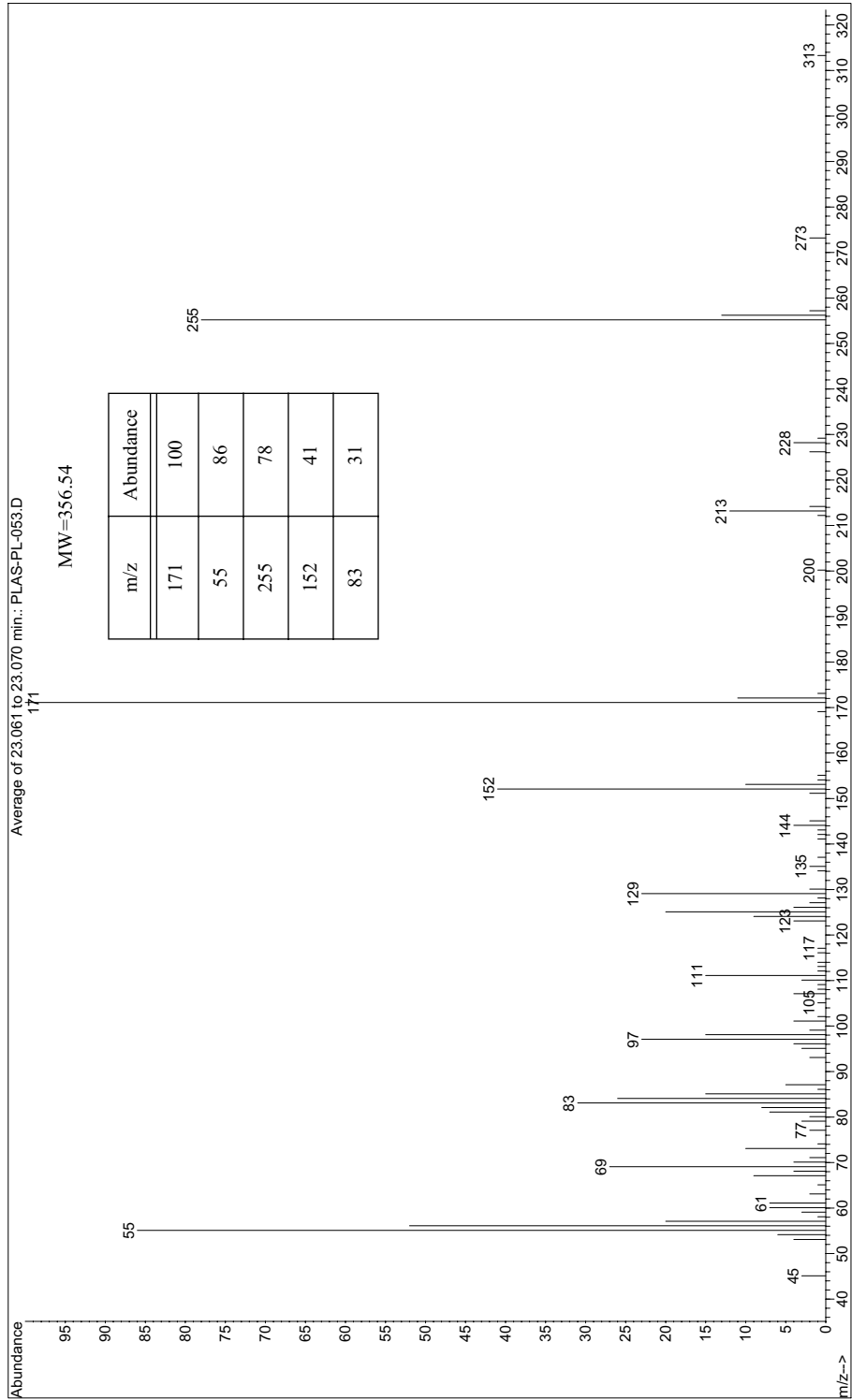
Point of Release

Can be released as point source pollution during manufacture, transportation, and final product end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

(LD50): 8.7–9.1 g/kg BW [Rat] and 11.5 g/kg BW [Mouse].

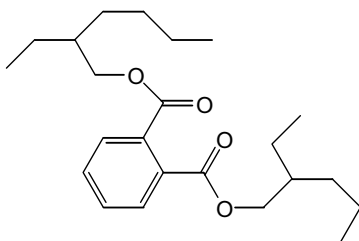
Mass Spectrum for *Plastolein 9050 - PLAS-PL-053*



For Chromatogram See Appendix A - PLAS-PL-053 - page 587

Polycizer® 162

Harwick Chemical Corporation

**CAS Number** 117-84-0**RTECS Number** TI1925000**Abbreviation** DNOP**Formula** C₂₄H₃₈O₄**Molecular Weight** 390.56**Chemical Name**

1,2-benzenedicarboxylic acid, dioctyl ester

Synonyms

di-N-octyl phthalate; dioctyl phthalate; dioctyl o-benzenedicarboxylate; dicapryl phthalate

Brand Names & Manufacturers

Polycizer 162

Harwick Chemical Corporation

Physical Properties**Appearance** Clear, colorless, viscous liquid**Melting Point** 25 °C**Boiling Point** 384 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	U	40-80	40-80	1-10

Application, Regulatory & Environmental Information

Application Used to keep plastics soft and more flexible. This type of plastic can be used for medical tubing and blood storage bags, wire and cables, carpet back coating, floor tile, and adhesives. It is also used in cosmetics and pesticides.

Regulatory Information

This chemical is considered to be an environmental hazard and regulated by the EPA under the Clean Water Act. It does have FDA approval for food contact applications.

Environmental Impact

If di-n-octylphthalate is released into the air, it may be deposited on the ground or to surface water in rain or dust particles. Di-n-octylphthalate sticks tightly to soil, sediment, and dust particles. Small amounts of di-n-octylphthalate can build up in animals that live in water, such as fish and oysters.

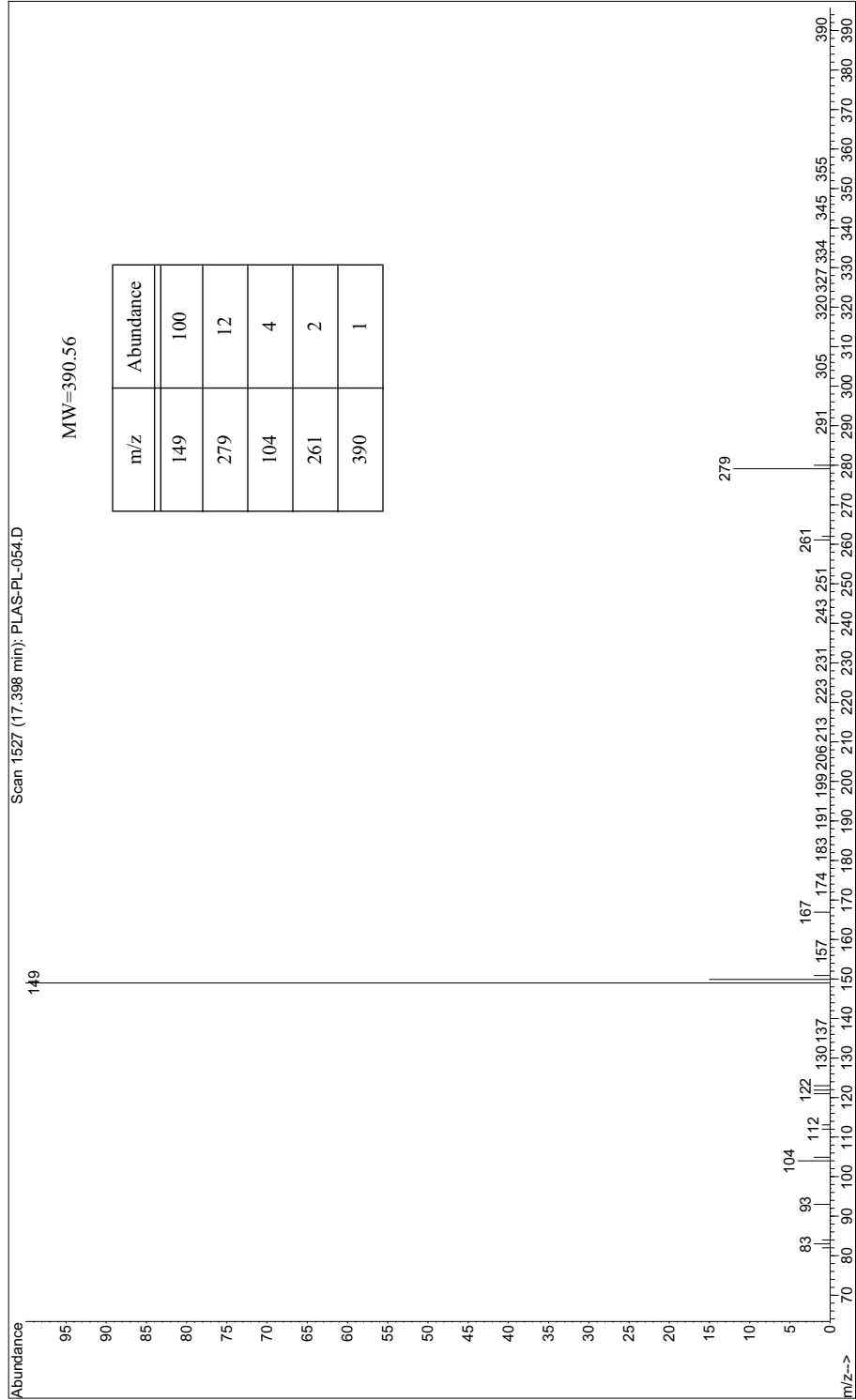
Point of Release

Exposure to di-n-octylphthalate occurs mainly from eating food or drinking water that is stored in plastic containers. This substance has been found in at least 300 of the 1416 National Priorities List sites identified by the Environmental Protection Agency (EPA). Di-n-octylphthalate can be released to water or air during its manufacture, by leaking from plastics in landfills, or from the burning of plastic products.

Toxicological Data

Di-n-octylphthalate has not been classified as to its carcinogenicity by the Department of Health and Human Services (DHHS) or the International Agency for Research on Cancer (IARC).

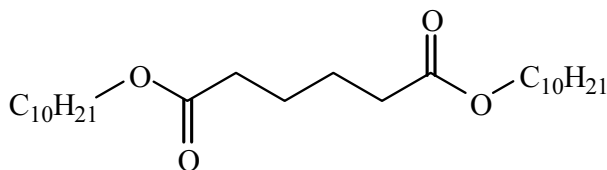
Mass Spectrum for Polycizer® 162 - PLAS-PL-054



For Chromatogram See Appendix A - PLAS-PL-054 - page 588

Polcizer® 632

Harwick Chemical Corporation

**CAS Number** 105-97-5**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₆H₅₀O₄**Molecular Weight** 426.67**Chemical Name**

hexanedioic acid, didecyl ester

Synonyms

didecyl hexanedioate; didecyl adipate; adipic acid didecyl ester

Brand Names & Manufacturers

Polcizer 632

Harwick Chemical Corporation

Physical Properties**Appearance** Light-colored liquid**Melting Point** N/A**Boiling Point** 245 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Plasticizer used in production of PVC, ethyl and nitrocellulose, polystyrene, and synthetic rubber intended for contact with food and drink.

Regulatory Information

Didecyl adipate is FDA approved under 21CFR177.2600 — Rubber articles intended for repeated use.

Environmental Impact

Readily biodegradable and has a low potential to bioaccumulate. Not expected to be toxic to the aquatic environment.

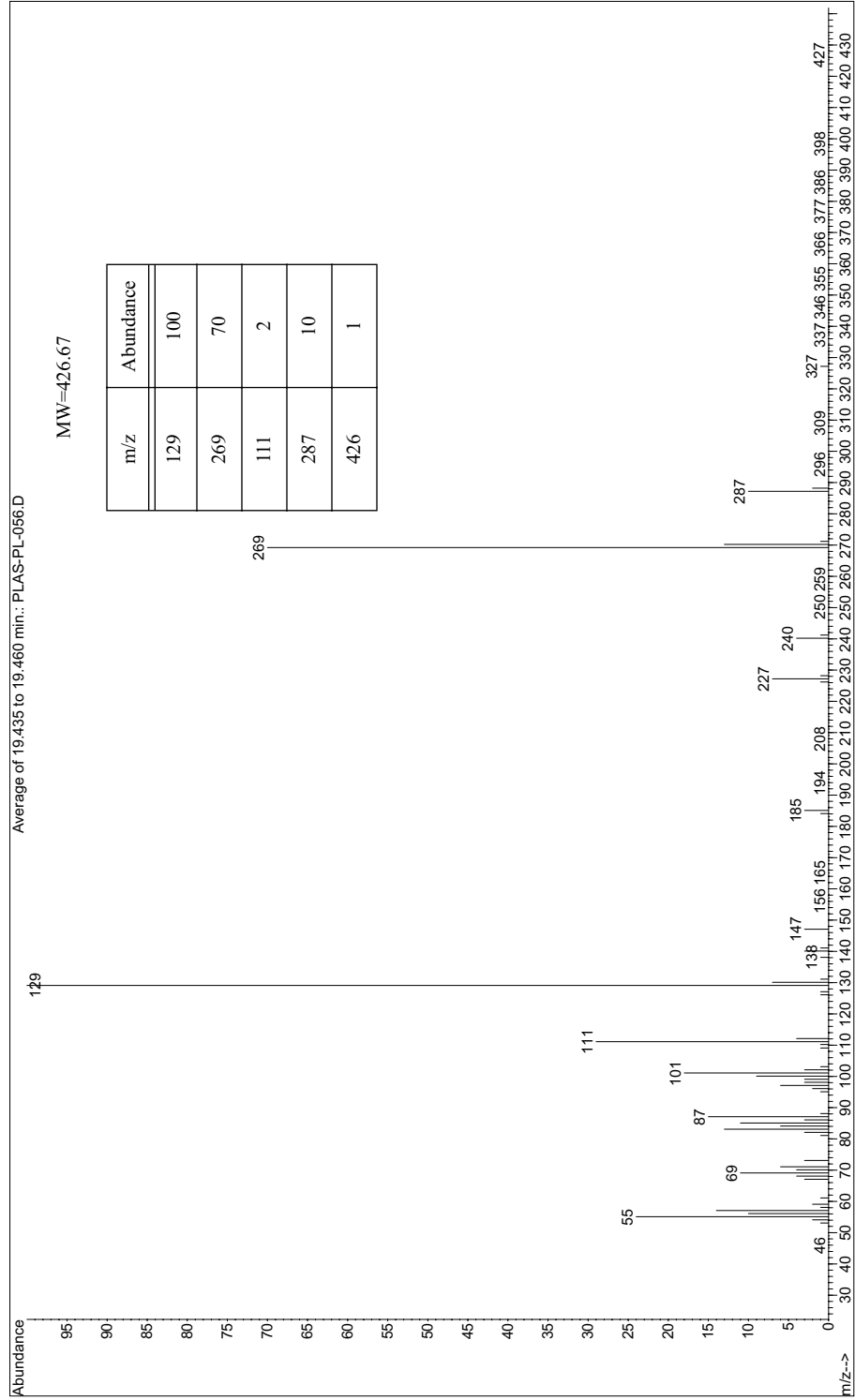
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

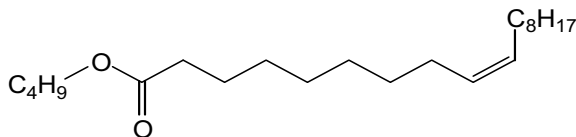
Mass Spectrum for Polycizer® 632 - PLAS-PL-056



For Chromatogram See Appendix A - PLAS-PL-056 - page 589

Polycizer® butyl oleate

Harwick Chemical Corporation

**CAS Number** 142-77-8**RTECS Number** RG3711000**Abbreviation** Not Identified**Formula** C₂₂H₄₂O₂**Molecular Weight** 338.57**Chemical Name**

butyl oleate

Synonyms

butyl cis-9-octadecenoate; oleic acid butyl ester

Brand Names & Manufacturers

Kessco® 554

Stepan Company

Vinicizer® 30

Kao Corporation

Witcizer 100

Physical Properties**Appearance** Off-white liquid**Melting Point** -26.4 °C**Boiling Point** 222.78°C @ 760 mm Hg**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 40-80	EtOH 40-80	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Plasticizer particularly for natural and synthetic rubber polymers. Used to impart a low temperature flexibility to neoprene formulations. Also used in cosmetics.

Regulatory Information

This product does not have FDA approval for direct or indirect food contact. It is not considered to be hazardous for shipping purposes, but is considered a primary irritant.

Environmental Impact

Possibly hazardous short-term degradation products are not likely. However, long-term degradation products may arise.

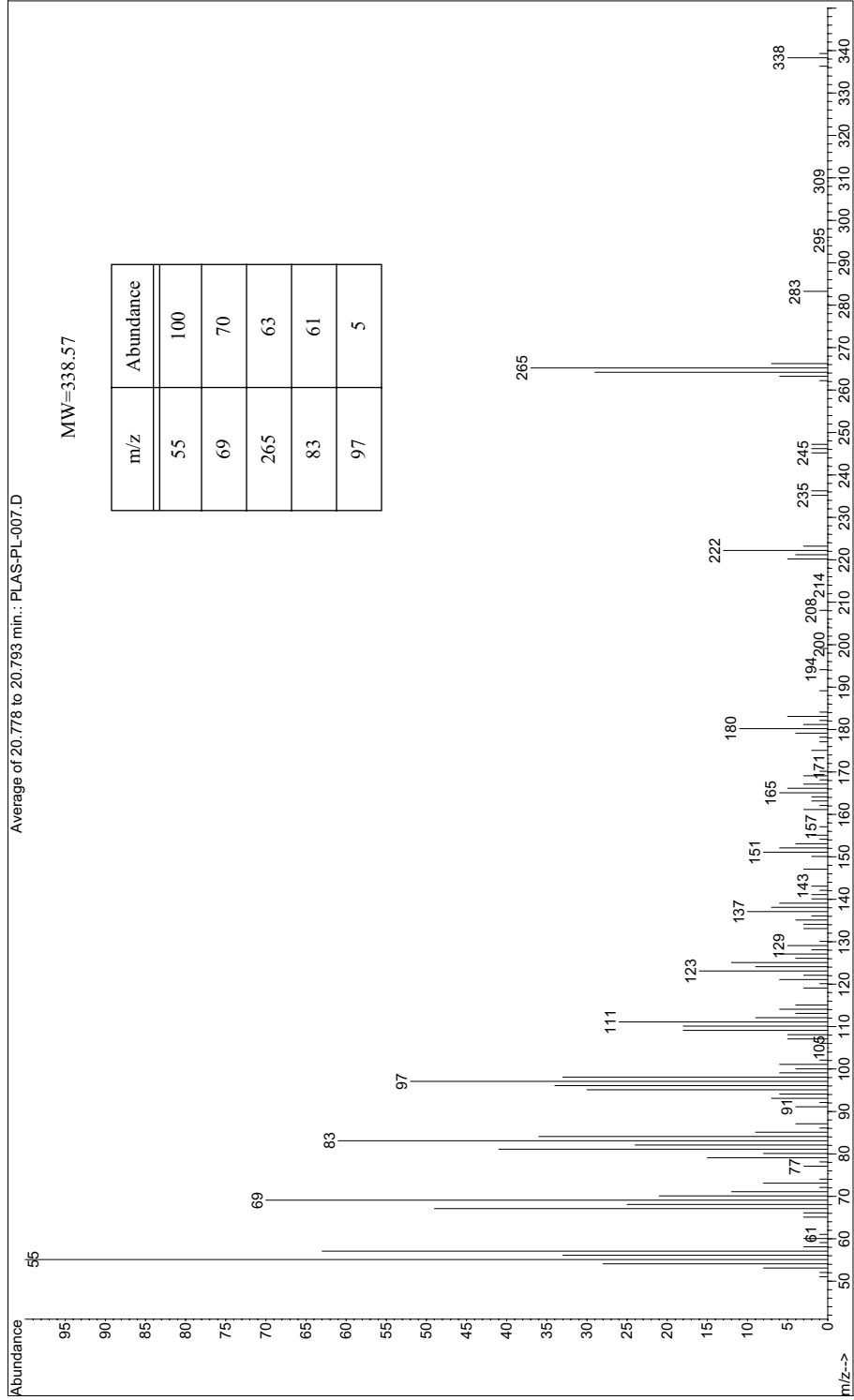
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

The product itself and its products of degradation are not toxic. It is considered to be hazardous in case of skin contact (irritant), inhalation (lung irritant), and slightly hazardous in case of ingestion. It is not classified as a carcinogen by IARC, NTP, or OSHA.

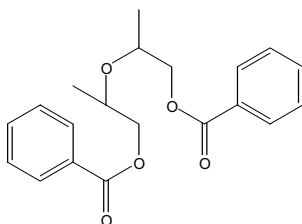
Mass Spectrum for Polycizer® butyl oleate - PLAS-PL-007



For Chromatogram See Appendix A - PLAS-PL-007 - page 590

Polycizer® DP 500

Harwick Chemical Corporation

**CAS Number** 27138-31-4**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₀H₂₂O₅**Molecular Weight** 342.39**Chemical Name**

dipropylene glycol dibenzoate

Synonyms

PPG-2 dibenzoate; oxybispropanol dibenzoate

Brand Names & Manufacturers

Benzoflex® 9-88

Velsicol Chemical Corporation

Santicizer® 9100

Ferro

Physical Properties**Appearance** Colorless to straw-colored liquid**Melting Point** <16 °C**Boiling Point** 232 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<0.1	U	U	40-80	40-80

Application, Regulatory & Environmental Information

Application Used in adhesives for the following applications: in the packaging industry for carton sealing/forming; for book binding and labeling; in textiles for both fibers and nonwoven fabrics; in construction to form decorative wall paneling, window frames, and other decorative construction products as well as producing mastics and caulking compounds. Also used in furniture, luggage, shoes, and cigarette tipping.

Regulatory Information

FDA approved for food contact under 21CFR175.105, 176.170, and 176.180. Regulated as an environmentally hazardous substance by DOT.

Environmental Impact

Toxic to aquatic organisms and may cause long-term adverse effects in the aquatic environment. Considered readily biodegradable.

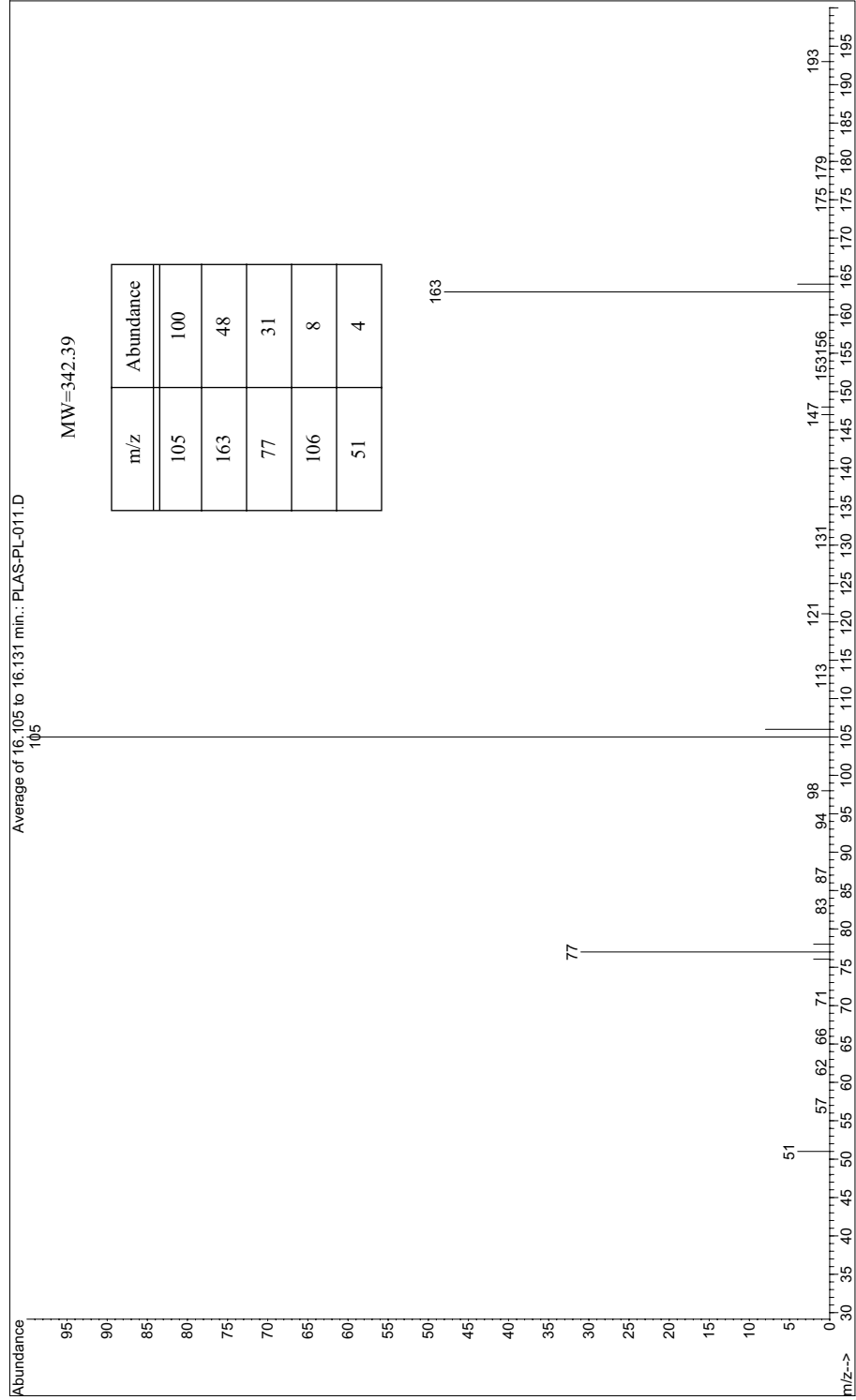
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

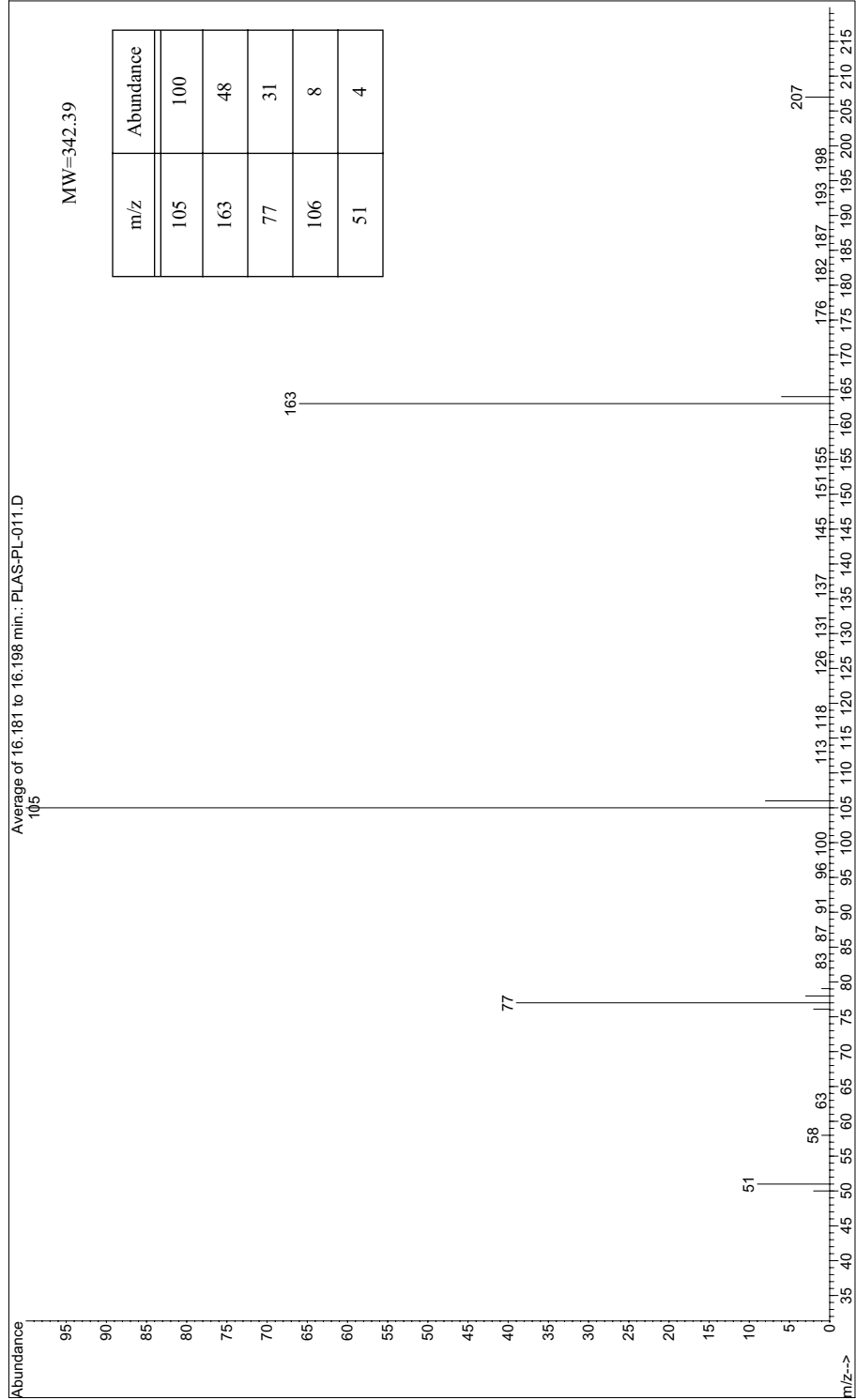
Acute oral toxicity (LD50): 9800 mg/kg [Rat].

Mass Spectrum for Polycizer® DP 500 - PLAS-PL-011



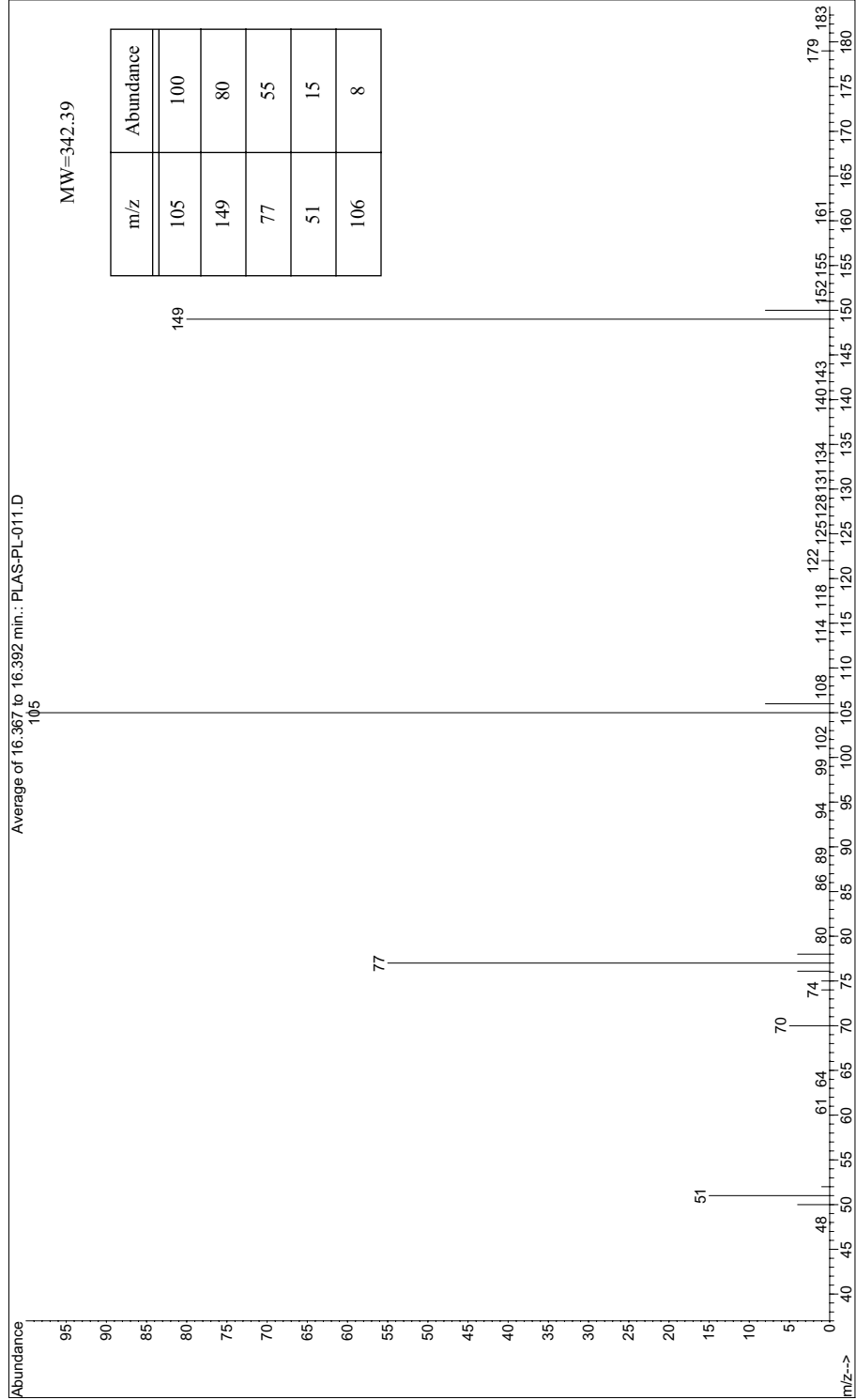
For Chromatogram See Appendix A - PLAS-PL-011 - page 591

Mass Spectrum for Polycizer® DP 500 - PLAS-PL-011



For Chromatogram See Appendix A - PLAS-PL-011 - page 591

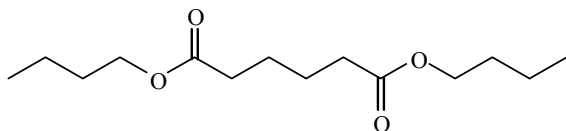
Mass Spectrum for Polycizer® DP 500 - PLAS-PL-011



For Chromatogram See Appendix A - PLAS-PL-011 - page 591

Polycizer® W 260

Harwick Chemical Corporation

**CAS Number** 105-99-7**RTECS Number** AV0900000**Abbreviation****Formula** C₁₄H₂₆O₄**Molecular Weight** 258.35**Chemical Name**

hexanedioic acid, dibutyl ester

Synonyms

dibutyl adipate; adipic acid, dibutyl ester

Brand Names & Manufacturers

Adimoll® DB

Bayer/Lanxess

Physical Properties**Appearance** Clear liquid**Melting Point** -32.4 °C**Boiling Point** 305 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application Used as low-temperature-resistant and low-viscosity plasticizer for PVC and its copolymers and cellulose esters, for example, cellulose acetate butyrate, and cellulose propionates. May be found in eyeglass frames, safety goggles, animal collars, decorative trims, and various types of film.

Regulatory Information

Dibutyl adipate is on the FDA GRAS (generally approved as safe) list.

Environmental Impact

Dibutyl adipate is readily biodegradable. Although it is considered to be moderately toxic to fish and daphnids and slightly toxic to algae, the environmental risk is considered to be low. Log Pow is 4.17, indicating that there is a moderate to low potential for bioaccumulation.

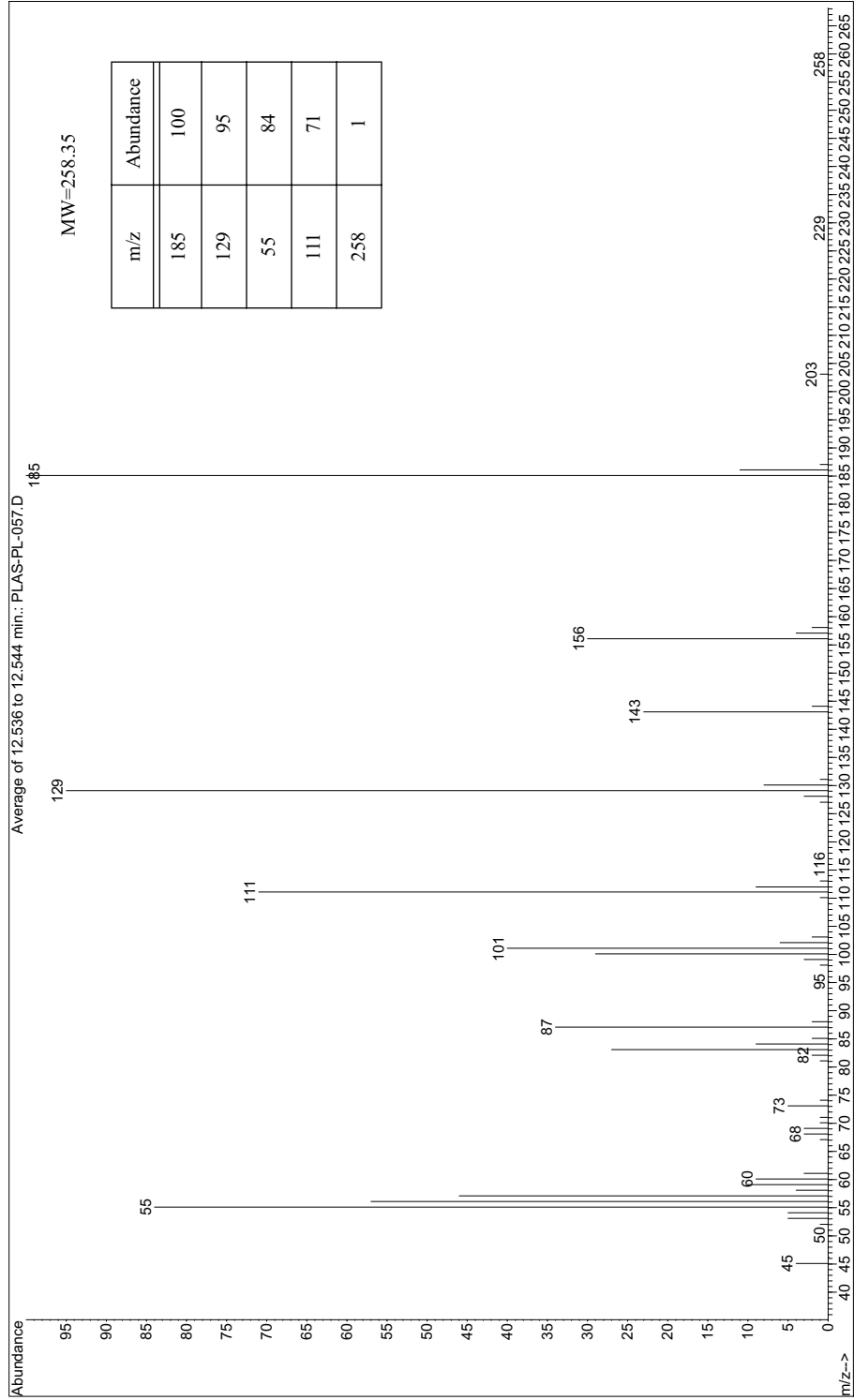
Point of Release

Primary exposure to dibutyl adipate is from skin contact with cosmetics and sunscreens containing this compound. It can also migrate from resins using this material as a plasticizer during the life cycle of the product and after disposal.

Toxicological Data

Dibutyl adipate is not toxic in acute oral or dermal animal toxicity tests.

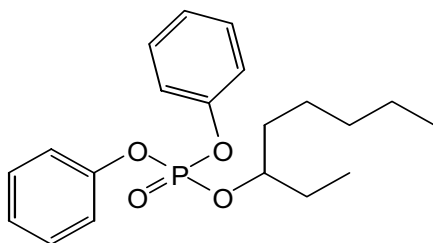
Mass Spectrum for Polycizer® W 260 - PLAS-PL-057



For Chromatogram See Appendix A - PLAS-PL-057 - page 592

Santicizer® 141

Solutia Inc.

**CAS Number** 1241-94-7**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₀H₂₇O₄P**Molecular Weight** 362.40**Chemical Name**

2-ethylhexyldiphenyl phosphate

Synonyms

phosphoric acid, 2-ethylhexyl diphenyl ester; diphenyl-2-ethylhexyl phosphate

Brand Names & Manufacturers

Santicizer 141

Solutia Inc.

Physical Properties**Appearance** Clear to yellow liquid**Melting Point** -80 °C**Boiling Point** 239 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	10-40	10-40	10-40	10-40	10-40

Application, Regulatory & Environmental Information

Application Flame retarding plasticizer used in cellulose, polyester, and polyurethane. Mainly used in the manufacture of electrical (wire and cable) and automotive plastic parts. May also be used for the preparation of vinyl sheets, fabric coating, plastisols and organosols, adhesives, vinyl packing materials, and conveyor belts.

Regulatory Information

FDA approved for indirect food contact.

Environmental Impact

Highly toxic to fish and aquatic plants. Has the potential to bioaccumulate and is not readily biodegradable.

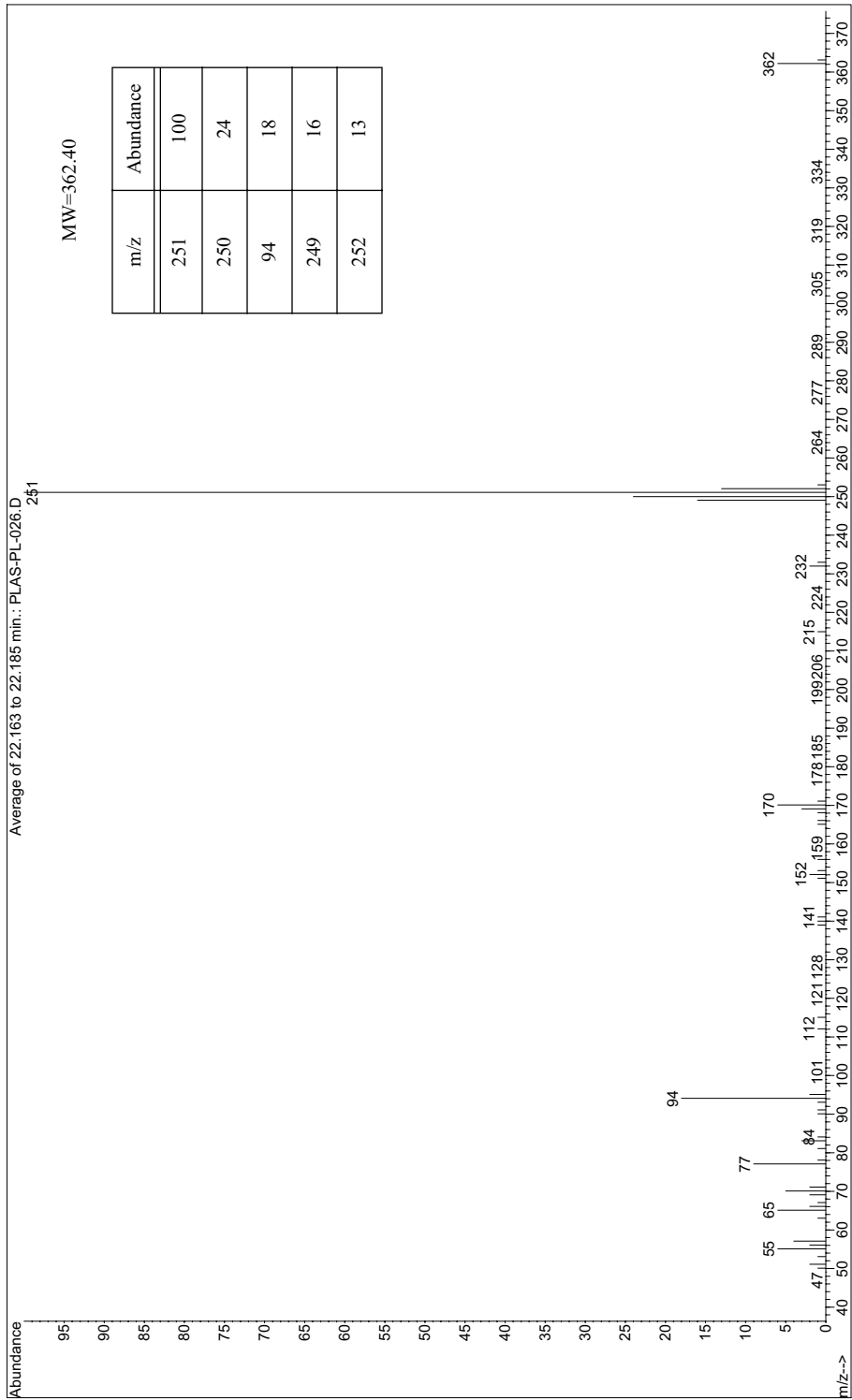
Point of Release

Organic phosphates are not chemically bonded to the polymer but can move in and out of the material. Evaporation of organic phosphates from car seats can result in a tacky coating on windows and other surfaces in the interior of the automobile, which can result in human exposure by skin contact and inhalation.

Toxicological Data

Acute oral (LD50): 218 mg/kg [Rabbit]; acute dermal (LD50): >7900 mg/kg [Rabbit].

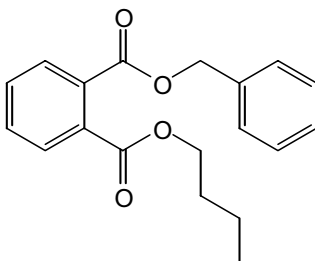
Mass Spectrum for Santicizer® 141 - PLAS-PL-026



For Chromatogram See Appendix A - PLAS-PL-026 - page 593

Santicizer® 160

Solutia Inc.

**CAS Number** 85-68-7**RTECS Number** TH9990000**Abbreviation** Not Identified**Formula** C₁₉H₂₀O₄**Molecular Weight** 312.37**Chemical Name**

benzyl butyl phthalate

Synonyms

1,2-benzenedicarboxylic acid, butyl phenylmethyl ester; butyl benzyl phthalate

Brand Names & Manufacturers

Palatinol® BB

BASF

Physical Properties**Appearance** Colorless, oily liquid**Melting Point** <-35 °C**Boiling Point** 370 °C**Stability** Stable under recommended storage and handling conditions.

Solubility	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
(g/100mL 20 °C)	<0.1	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Butyl benzyl phthalate is a plasticizer added to polymers to give flexibility and softness. It is used extensively in polyvinyl chloride and in cellulose plastics, polyvinyl acetate, polysulfides, and polyurethane. Also used in flexographic inks for food packaging applications and acrylic coatings, profile extrusions, slush molding, film and sheeting, coated fabrics, floor and wall coverings, vinyl foams, and plastisols for car sealants.

Regulatory Information

Considered a priority pollutant and is regulated by the federal Clean Water Act, RCRA, and Superfund. FDA approved under 21CFR175.105 — Adhesives; 175.300 — Resinous and Polymeric Coatings; 176.170 — Components of Paper & Paperboard in Contact with Fatty or Aqueous Food; 175.180 — Components of Paper & Paperboard in Contact with Dry Food; 177.2420 — Cross-linked Polyester Resins (as solvent); and 178.3740 — Polymeric Substances (Extraction limitations).

Environmental Impact

This substance is very toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish.

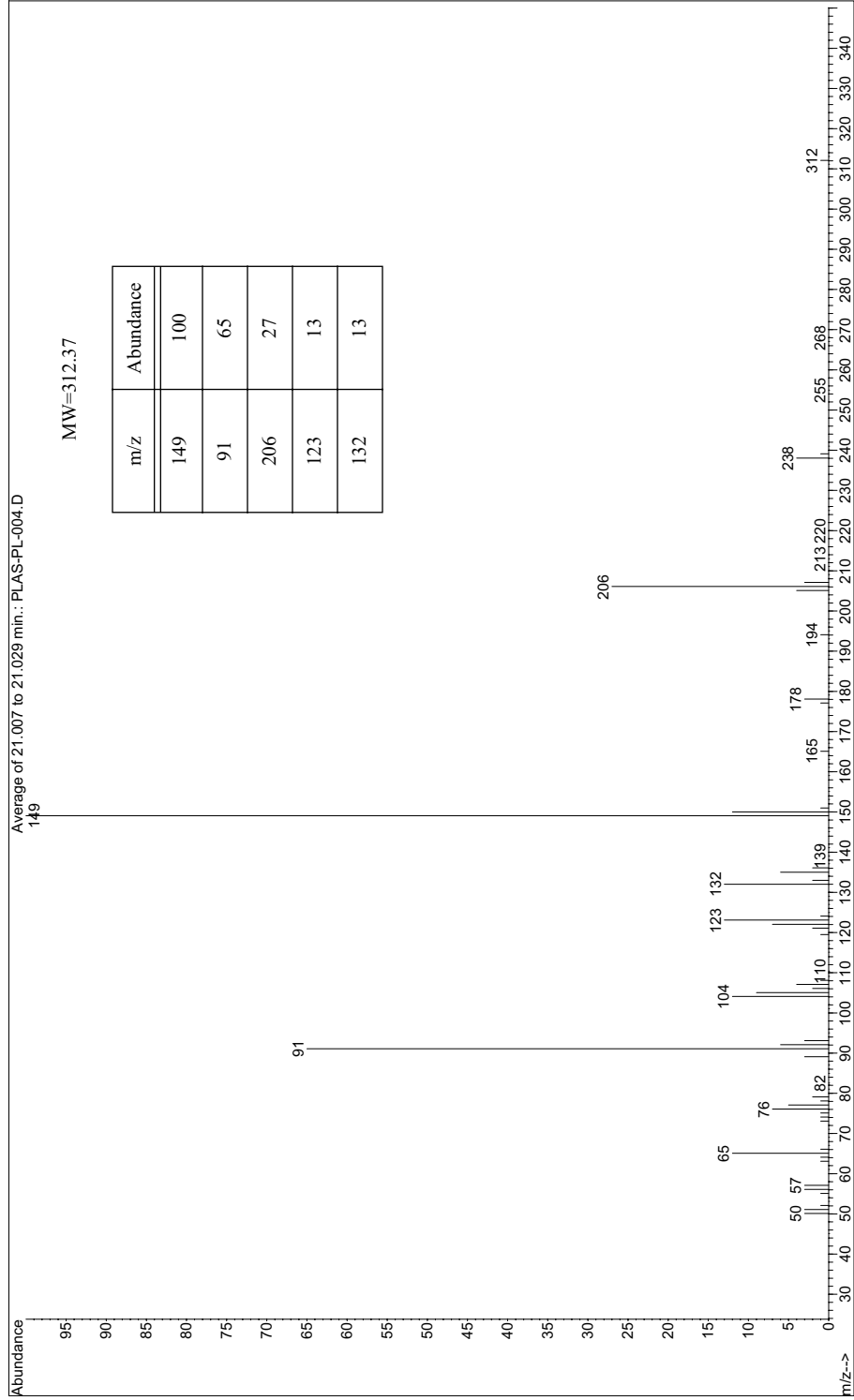
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Tumorigen; mutagen; reproductive effector. acute oral toxicity (LD50): 2330 mg/kg [Rat]. Acute dermal toxicity (LD50): 6700 mg/kg [Rat]. Lowest published toxic oral dose (TDLo): 68250 mg/kg/91D-C [Rat]. State of California (Proposition 65) as known to cause reproductive toxicity.

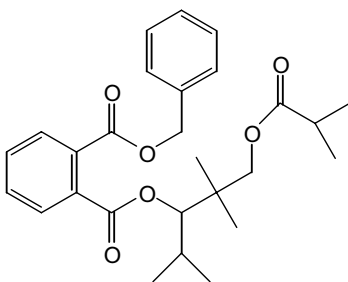
Mass Spectrum for Santicizer® 160 - PLAS-PL-004



For Chromatogram See Appendix A - PLAS-PL-004 - page 594

Santicizer® 278

Solutia Inc.

**CAS Number** 16883-83-3**RTECS Number** Not Available**Abbreviation** Not Identified**Formula** C₂₇H₃₄O₆**Molecular Weight** 454.56**Chemical Name**

benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate

Synonyms2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl-1,2-benzenedicarboxylic acid
phenylmethyl ester**Brand Names & Manufacturers**

Santicizer® 278

Solutia Inc.

Physical Properties**Appearance** Clear, oily liquid**Melting Point** N/A**Boiling Point** 243 °C (10 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
<0.1	U	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Santicizer 278 is used in PVC, acrylic coatings, polyurethanes, chlorinated rubber, butyl rubber, and polysulfides. It is a versatile plasticizer for use in many resin systems, from automobile sealants to water-blown methylene diisocyanate based polyurethane foams. Other applications include use as a yellowing inhibitor for thermoplastic polycarbonate resins exposed to gamma radiation and as a solvent for pressure-sensitive copying paper giving copies improved resistance to fading. It is also used for interlayers of sandwich glass for cars and buildings.

Regulatory Information

Not specifically listed in 21 CFR for use in food applications. When discarded, the compound is not a hazardous waste, as defined by the Resource, Conservation and Recovery Act (RCRA), and it is also not considered hazardous under the Department of Transportation (DOT) regulations. It is, however, listed in the Toxic Substances Control Act (TSCA) Inventory.

Environmental Impact

The EPA Registry classifies this compound as non-persistent, bioaccumulative, and inherently toxic to aquatic organisms.

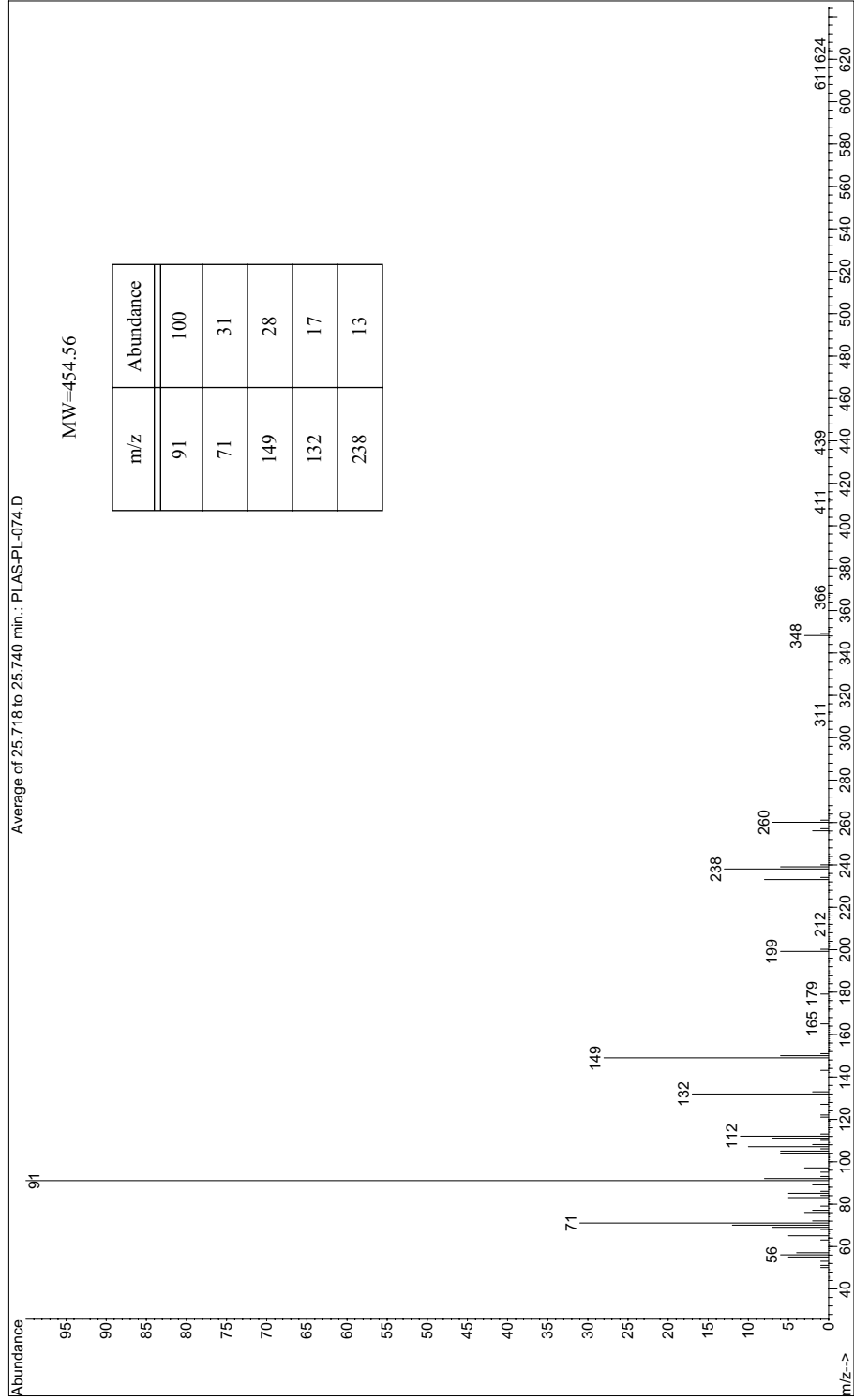
Point of Release

Phthalates are not chemically bound to the product and therefore may leach into the surrounding medium.

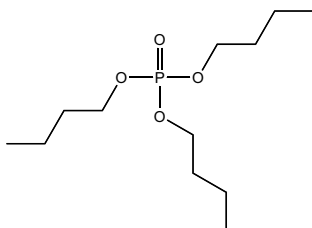
Toxicological Data

Acute oral toxicity (LD50): >15800 mg/kg [Rat]; acute dermal toxicity (LD50): >10000 mg/kg [Rabbit]. When applied to the skin and eyes of six rabbits for a period of 24 hours, was reported to be practically non-irritating.

Mass Spectrum for Santicizer® 278 - PLAS-PL-074



For Chromatogram See Appendix A - PLAS-PL-074 - page 595

Tributylphosphate

CAS Number 126-73-8
RTECS Number TC7700000
Abbreviation TBP

Formula C₁₂H₂₇O₄P
Molecular Weight 266.31

Chemical Name
tributyl phosphate

Synonyms
tri-n-butyl phosphate

Brand Names & Manufacturers

Disflamoll® TB

Lanxess

Physical Properties

Appearance Clear liquid

Melting Point -79 °C

Boiling Point 288-289 °C

Stability Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
0.6	S	S	U	U	S	

Application, Regulatory & Environmental Information

Application Used as an antifoaming agent in fuel, coating, papermaking, and oil drilling industries. It also can be used as a plasticizer for cellulose esters such as nitrocellulose and cellulose acetate.

Regulatory Information

Not FDA approved for food contact applications.

Environmental Impact

The substance is toxic to aquatic organisms. Fugacity Level III calculations indicate that if released into the environment, it will exist predominantly in the soil and/or the aquatic environment depending on the environmental compartment that they first contact. The log Kow indicates low bioaccumulation potential.

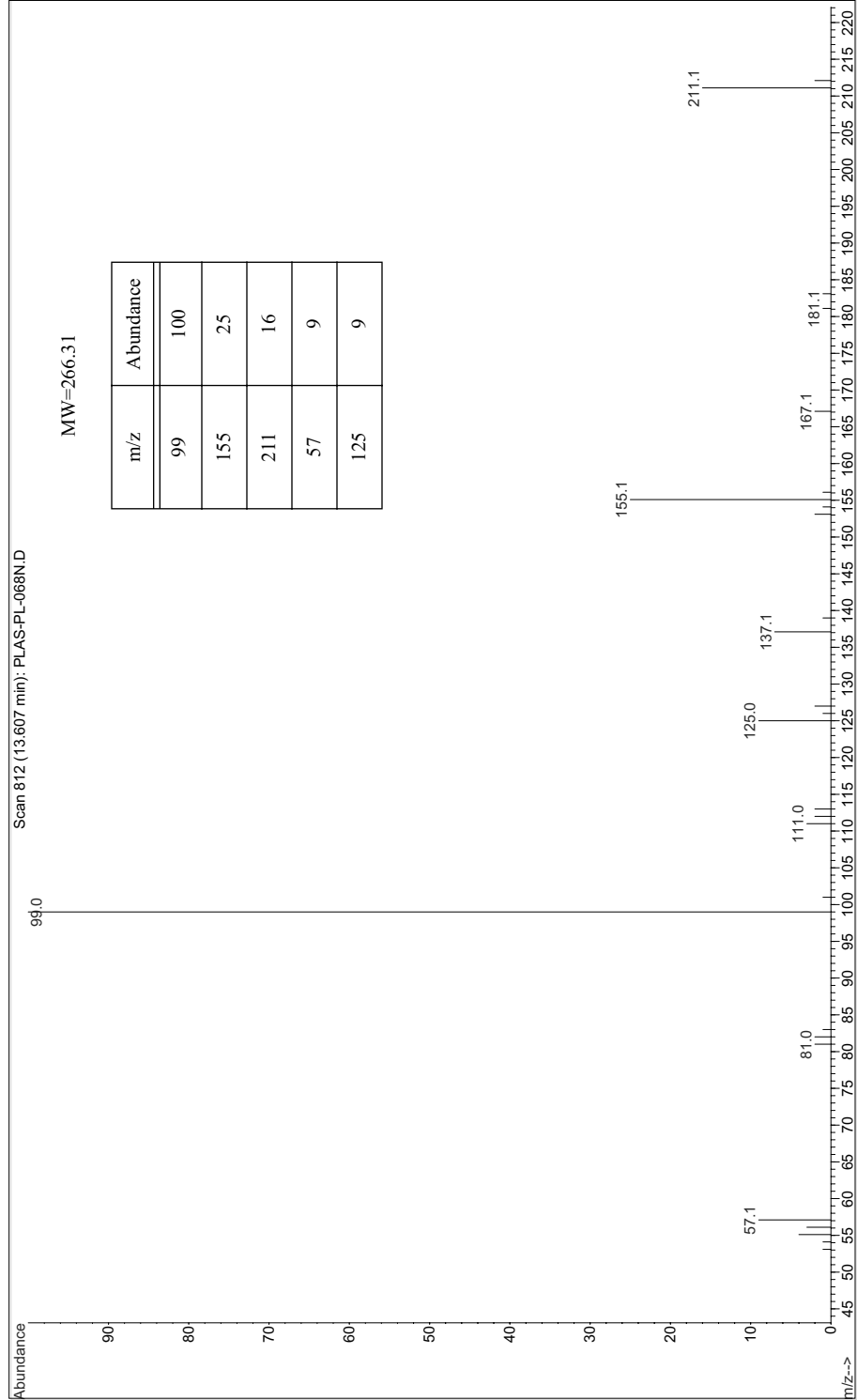
Point of Release

TBP has been identified in indoor air and drinking water. The general population may be exposed during use of the products it is used in.

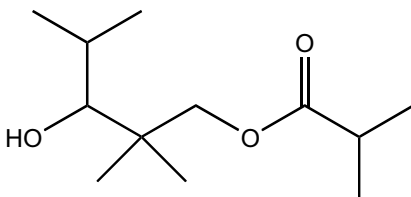
Toxicological Data

Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems. Repeated or prolonged exposures to cholinesterase inhibitors produce symptoms similar to acute effects. In addition, workers exposed repeatedly to these substances may exhibit impaired memory and loss of concentration, severe depression and acute psychosis, irritability, confusion, apathy, emotional liability, speech difficulties, headache, spatial disorientation, delayed reaction times, sleepwalking, drowsiness, or insomnia.

Mass Spectrum for Tributylphosphate - PLAS-PL-068



For Chromatogram See Appendix A - PLAS-PL-068 - page 596

2,2,4-Trimethyl-1,3-pentanediol-isobutyrate**CAS Number** 25265-77-4**RTECS Number** UF6000000**Abbreviation** Not Identified**Formula** C₁₂H₂₄O₃**Molecular Weight** 216.32**Chemical Name**

(3-hydroxy-2,2,4-trimethylpentyl) 2-methylpropanoate

Synonyms

2,2,4-Trimethyl-1,3-pentanediolmono(2-methylpropanoate)

Brand Names & Manufacturers

Texanol™

Eastman Chemical

Physical Properties**Appearance** Liquid**Melting Point** -50 °C**Boiling Point** 244 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water 0.086	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application**

Predominant use of this substance is as a coalescing aid at up to 3% concentration in latex paints. Also used as a chemical intermediate which is converted to other chemical substances used as plasticizers. May also be found in dyestuffs, adhesives, building material agents, detergents, cleaning agents, and fertilizers.

Regulatory Information

Not FDA approved for food contact.

Environmental Impact

Based on its physiochemical properties, the test material will not be a persistent environmental contaminant. Little to no potential for bioaccumulation exists.

LC50 96 hour: >19 mg/L [Fish].

Point of Release

Environmental exposure occurs primarily through volatilization of the substance from drying latex paint. Terrestrial and aquatic exposure would occur rarely through spills. The substance is predicted to undergo photodecomposition slowly in the atmosphere, and does not persist elsewhere in the environment because it biodegrades at a modest rate.

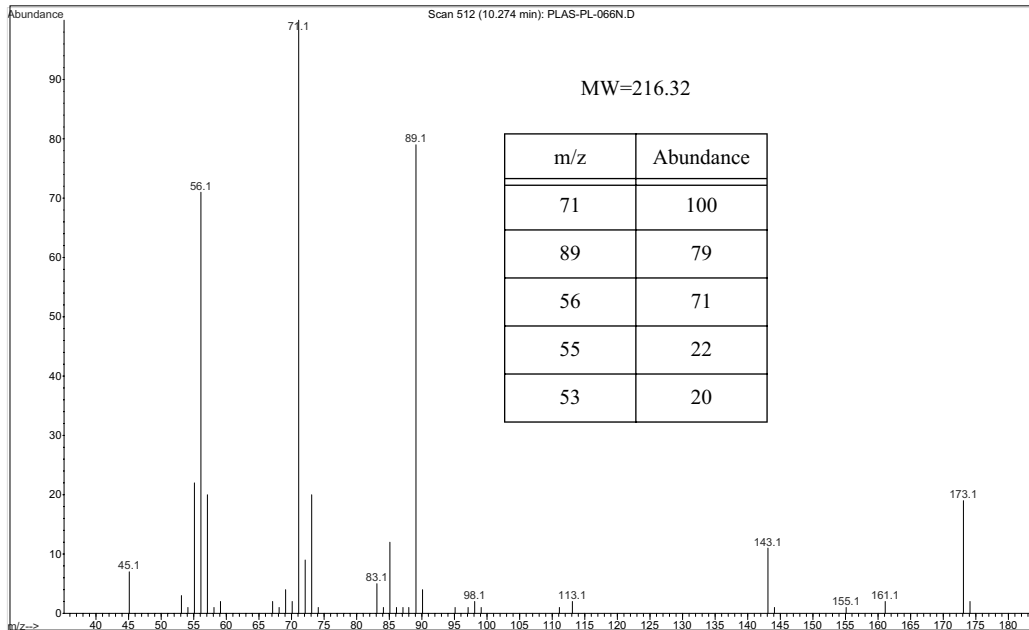
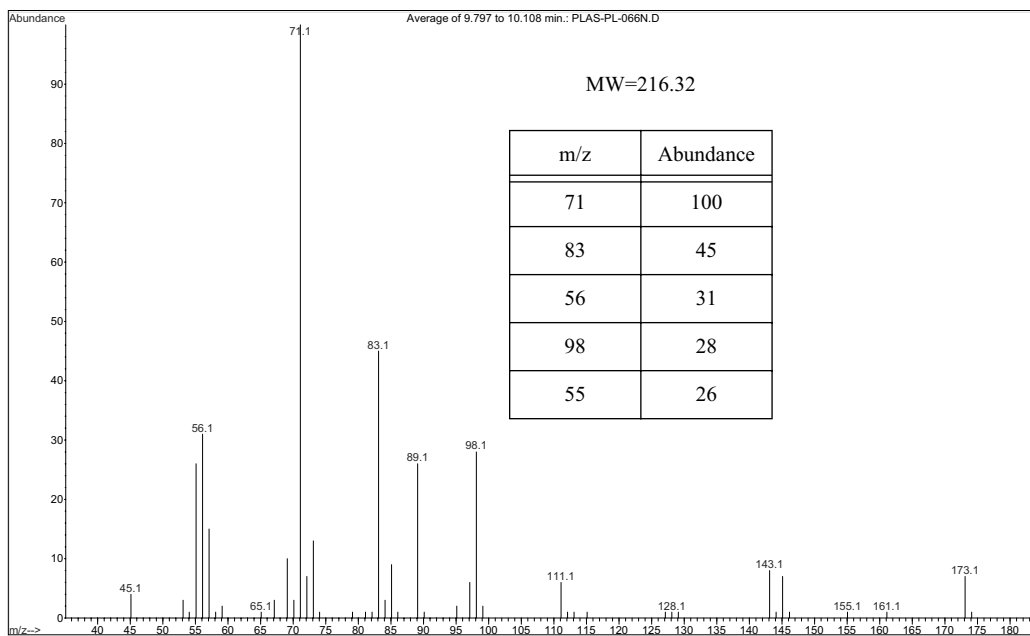
Toxicological Data

The results of the SIDS testing indicate that the substance has a relatively low order of toxicity.

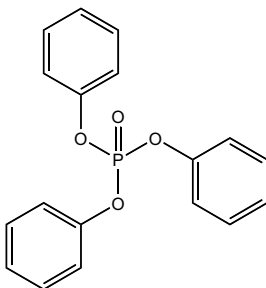
LD50 Oral: 6517 mg/kg [Rat].

LC50 Inhalation: 1600–3200 mg/kg [Rat].

LD50 Dermal: >16 ml/kg [Guinea Pig].

Mass Spectra for 2,2,4-Trimethyl-1,3-pentanediol-isobutyrate - PLAS-PL-066

For Chromatogram See Appendix A - PLAS-PL-066 - page 597

Triphenylphos-**CAS Number** 115-86-6**RTECS Number** TC8400000**Abbreviation** TPP**Formula** C₁₈H₁₅O₄P**Molecular Weight** 326.28**Chemical Name**

triphenyl phosphate

Synonyms

phosphoric acid triphenyl ester

Brand Names & ManufacturersCelluflex[®] TPP

Celanese Corporation of America

Disflamoll[®] TP

Lanxess

Phosflex[®] TPP

Supresta

Physical Properties**Appearance** White flakes or powder**Melting Point** 49-50 °C**Boiling Point** 245 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH S	EtOH S	Acetone S	CH₂Cl₂ U	Hexane U
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Application *Application, Regulatory & Environmental Information*

Used as a plasticizer and fire retardant primarily for flexible PVC applications such as artificial leather. Other applications include coatings, as carriers for pigment dispersions, leveling agents for floor finishes, and as plasticizing additives for elastomers. It is also used as a plasticizer in the production of cellulose acetate films.

Regulatory Information

Not FDA approved for food contact applications.

Environmental Impact

LC50 (96 h): 0.4 mg/l [Fish].

EC50 (48 h): 1.0 mg/l [Invertebrate].

BCF: 110–114 [Fish].

Point of Release

The general population may be exposed during use of the products it is used in.

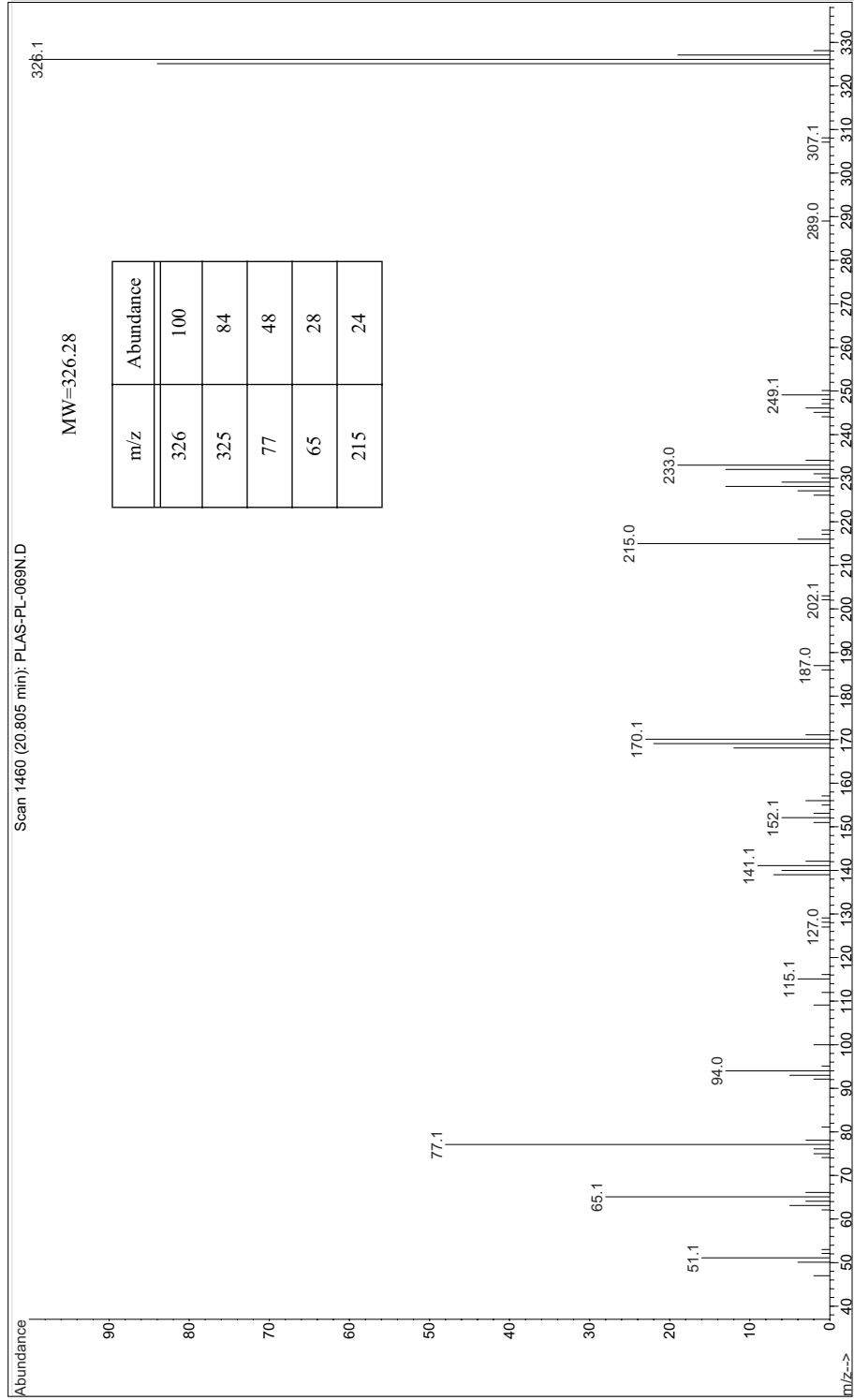
Toxicological Data

LD50 (oral): 3500 mg/kg [Rat].

LD50 (oral): 1320 mg/kg [Mouse].

LD50 (dermal): >7900 mg/kg [Rabbit].

Mass Spectrum for Triphenylphosphate - PLAS-PL-069



For Chromatogram See Appendix A - PLAS-PL-069 - page 598

Vinsol® resin

Pinova

Unspecified Structure

CAS Number 8050-09-7

RTECS Number VL0480000

Abbreviation Not Identified

Formula Unspecified

Molecular Weight N/A

Chemical Name

gum rosin

Synonyms

disproportionated rosin; polymerized rosin; colophony

Brand Names & Manufacturers

Vinsol resin

Pinova

Physical Properties

Appearance Dark reddish-brown solid**Melting Point** 75-81 °C**Boiling Point** >572 °C**Stability** Stable under recommended storage and handling conditions.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	<0.1

Application, Regulatory & Environmental Information

Application

Used as an air entraining agent in cements, mortars, and concrete to improve strength, workability, and freeze/thaw resistance. Also used as an asphalt emulsifier for anionic, slow setting emulsions for paving, surfacing, and sealing applications. Other uses include adhesives, sealants, inks, coatings, binder in paperboard and composition board, foundry molds, and core washes.

Regulatory Information

FDA approved for a wide range of applications ranging from direct food additives such as chewing gum base to indirect food additives in adhesives, paper and paperboard, and polymers as per 21CFR175, 176, 177, and 178.

Environmental Impact

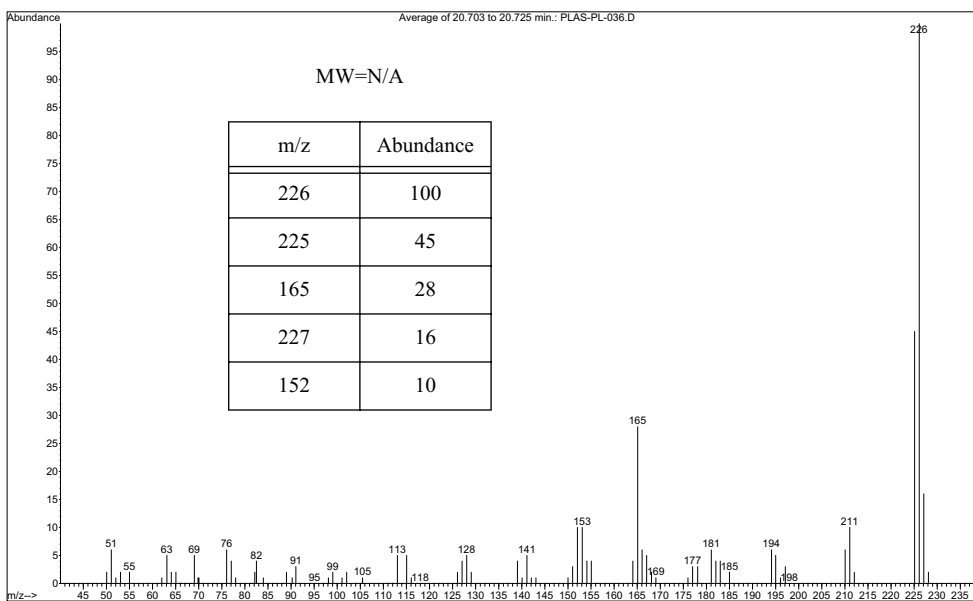
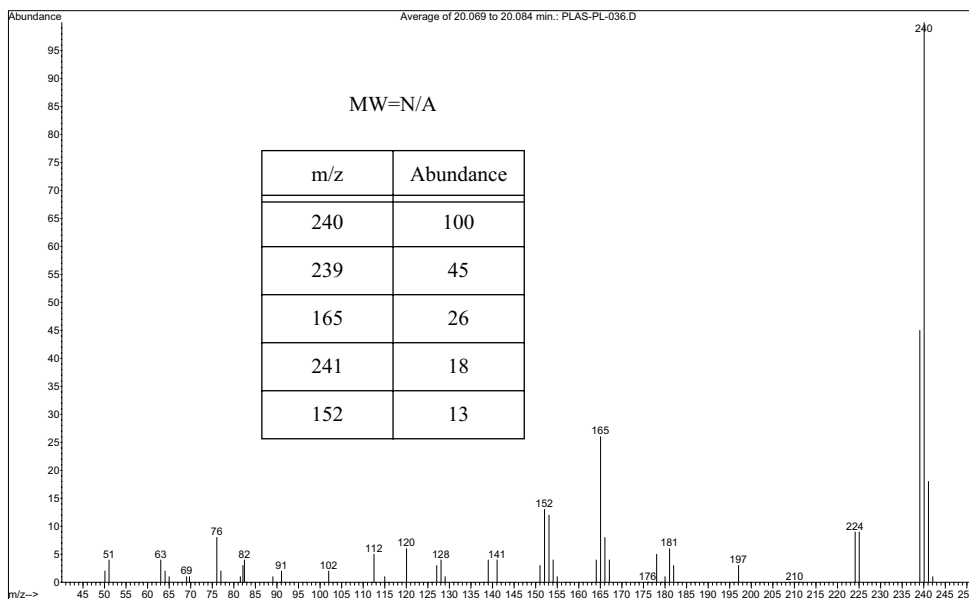
Based upon data from this or similar materials, this product cannot be regarded as readily biodegradable; however, it may be slowly biodegradable. Acute 96 hour (LL50): > 1000 mg/L [Fathead Minnow]. Acute 48 hour (EL50): 911 mg/L [Daphnia magna], algae growth inhibition test 72 hour (EL50): > 1000 mg/L.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

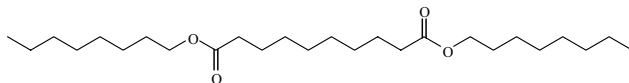
Not considered a carcinogen by OSHA, IARC, or NTP. Acute inhalation toxicity (LD50): 110 mg/m³ [Rat]. Acute oral toxicity (LD50): 2.2 mg/kg [Mouse], 3.0 mg/kg [Rat].

Mass Spectra for Vinsol[®] resin - PLAS-PL-036

For Chromatogram See Appendix A - PLAS-PL-036 - page 599

Witamol 500

Degussa

CAS Number 2432-87-3**RTECS Number** N/A**Abbreviation** DOS**Formula** C₂₆H₅₀O₄**Molecular Weight** 426.67**Chemical Name**

decanedioic acid, dioctyl ester

Synonyms

dioctyl sebacate; di-n-octyl sebacate; sebacic acid, dioctyl ester; dioctyl decanedioate

Brand Names & Manufacturers

Witamol 500

Degussa

Physical Properties**Appearance** Colorless liquid**Melting Point** -67 °C**Boiling Point** 300 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 40-80	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application Plasticizer for PVC, and its copolymers, nitrocelluloses, styrene resins, and synthetic rubbers where low temperature performance is required. The end applications include anti-frosting cable and PVC linoleum.

Regulatory Information

Di-n-octyl sebacate has FDA approval under 21CFR178.3910 — Surface Lubricants Used in the Manufacture of Metallic Articles.

Environmental Impact

Based on studies of isomers, this material is expected to be readily biodegradable. If released into the environment, it would be expected to partition into the soil and sediment. Bioaccumulation potential is low.

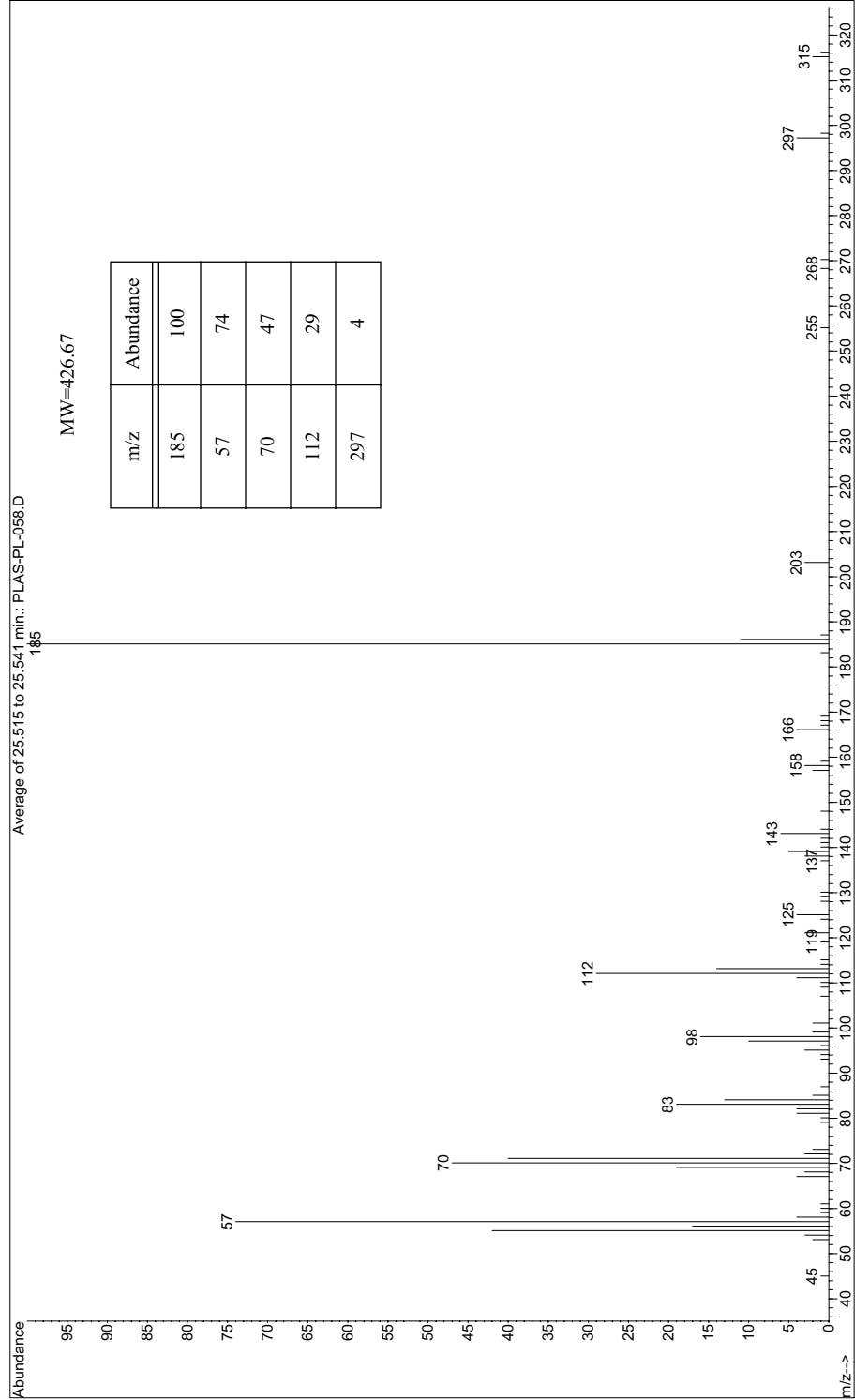
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral toxicity (LD50): 9500 mg/kg [Mouse]. Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectrum for Witamol 500 - PLAS-PL-058



For Chromatogram See Appendix A - PLAS-PL-058 - page 600

Other Compounds of Interest

This chapter contains information on additives such as processing aids, retarders, and stearates. While these compounds may not be as widely used as plasticizers or antioxidants, they play an important role in plastic and rubber processing.

Processing Aids

This group includes compounds that lower the viscosity of a polymer during processing without increasing the plasticizer level (viscosity depressants), parting agents applied to the surface of a mold to provide a release coating and prevent molded articles from sticking to the mold (mold-release agents), compounds added to provide additional stability by increasing internal adhesion in heterogeneous systems or emulsions (emulsifier/surfactants), modifiers used to provide lubrication during processing (slip agents), and preservatives added to prevent attack from fungi, bacteria, and yeast (antimicrobials) to name a few.

Crosslinking Retarders

Retarders are chemical compounds used to slow down the crosslinking process, primarily for sulfur-containing crosslinking agents for production of elastomeric products. These materials are added to prolong the flow time in a molding operation, for example, before the material becomes fully crosslinked. Elastomeric objects with high mass and a need for precision molded detail are typically treated with retarders. These are particularly effective where internal thermal gradients cannot be precisely controlled due to inherently poor thermal conductivity and the exothermic crosslinking reactions. Retarders that are most commonly used include stearic acid, benzoic acid, salicylic acid, and phthalic anhydride.

Stearates

This group includes salts and esters of stearic acid, which is a saturated fatty acid. Often termed as “metallic stearates”, these compounds are used as release agents in processing polyolefins, polystyrenes, polyesters, and rubbers.

Blowing Agents

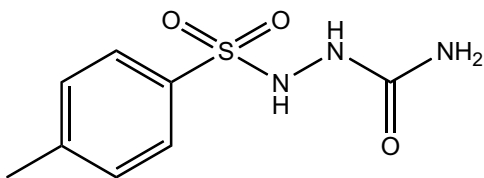
Organic compounds that evolve gaseous decomposition products upon moderate heating are often used in the production of polymeric and elastomeric foams. Some foams are formed in processes that involve direct injection of nitrogen gas in a closed process where a positive pressure can be held until crosslinking is initiated. Gas held in this manner expands and forms open or closed cell foam structures. Blowing agents were developed in the 1940s, initially for use with PVC. Most had undesirable toxicity. Safe organic blowing agents were developed and are most commonly used today for production of foams with controlled structures. Most of these compounds are azides such as azodicarbonamide, p-toluene sulfonyl hydrazide, and 5-phenyl tetrazole. Commercially available blowing agents are limited to approximately 15 different compounds. These are blended with a polymer compound and thermally initiated decomposition produces nitrogen gas. Depending on the type of blowing agent, initiation typically occurs for some at 120°C, with others decomposing at 250°C to 270°C.

Analytically, these compounds are typically a challenge to detect because they would fully decompose upon heating. However, complete consumption may be limited by the processing time during foam production, incomplete heat transfer, and the retarding effects of other additives.

Antistats

In many applications, accumulation of electric charge by polymers with a high dielectric constant presents an undesirable characteristic. Dust attraction on the surface of appliances and furniture are good indicators of an undesirable property of many polymers. The magnitude of static electric charge build-up can be controlled by addition of electrically active materials, including organic and inorganic ingredients. The latter include such components as metal powders, carbon black, and others, all of which are beyond the scope of this Handbook. There are a number of organic antistats that work by controlling either the surface charge or the bulk electric charge. Antistats typically have limited compatibility with the host polymer. Most feature polar and non-polar end groups. The limited compatibility forces the antistat to migrate to the free surface of a polymeric material. The polar groups react with water on the surface to produce a weakly conductive surface film. Sorbitol esters, such as Span and polyoxyethylene esters, such as Tween, have been in wide commercial use as antistats. Ethoxylated tertiary amines are also used for antistat applications.

From an analytical perspective, it is important to note that these materials are used in very low bulk concentration in most polymer applications. This avoids bulk adsorption into polymers. Analysis for antistats is best performed with sampling of the outermost surface.

Celogen® RA**CAS Number** 10396-10-8**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₈H₁₁N₃O₃S**Molecular Weight** 229.26**Chemical Name**

((4-methylphenyl)sulfonylamino)urea

Synonyms

p-toluenesulfonyl semicarbazide

Brand Names & Manufacturers

Mikrofine TSSC

Geon Corporation

Physical Properties**Appearance** White crystals**Melting Point** 227-230 °C**Boiling Point** N/A**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	U	<0.01	U	<0.01

Application *Application, Regulatory & Environmental Information*

Used as a foaming agent for expanded plastics and sponge rubber at high processing temperature. Can be used in combination with very strong activators such as treated urea, moderate activators such as barium stearate, calcium stearate, zinc stearate, and zinc oxide. Can be used in plastics such as ABS polymers, rigid polyvinyl chloride, high density polyethylene and polypropylene, natural, SBR, BR, nitrile, neoprene, EPDM, and butyl rubbers.

Regulatory Information

Not FDA approved for food contact applications.

Environmental Impact

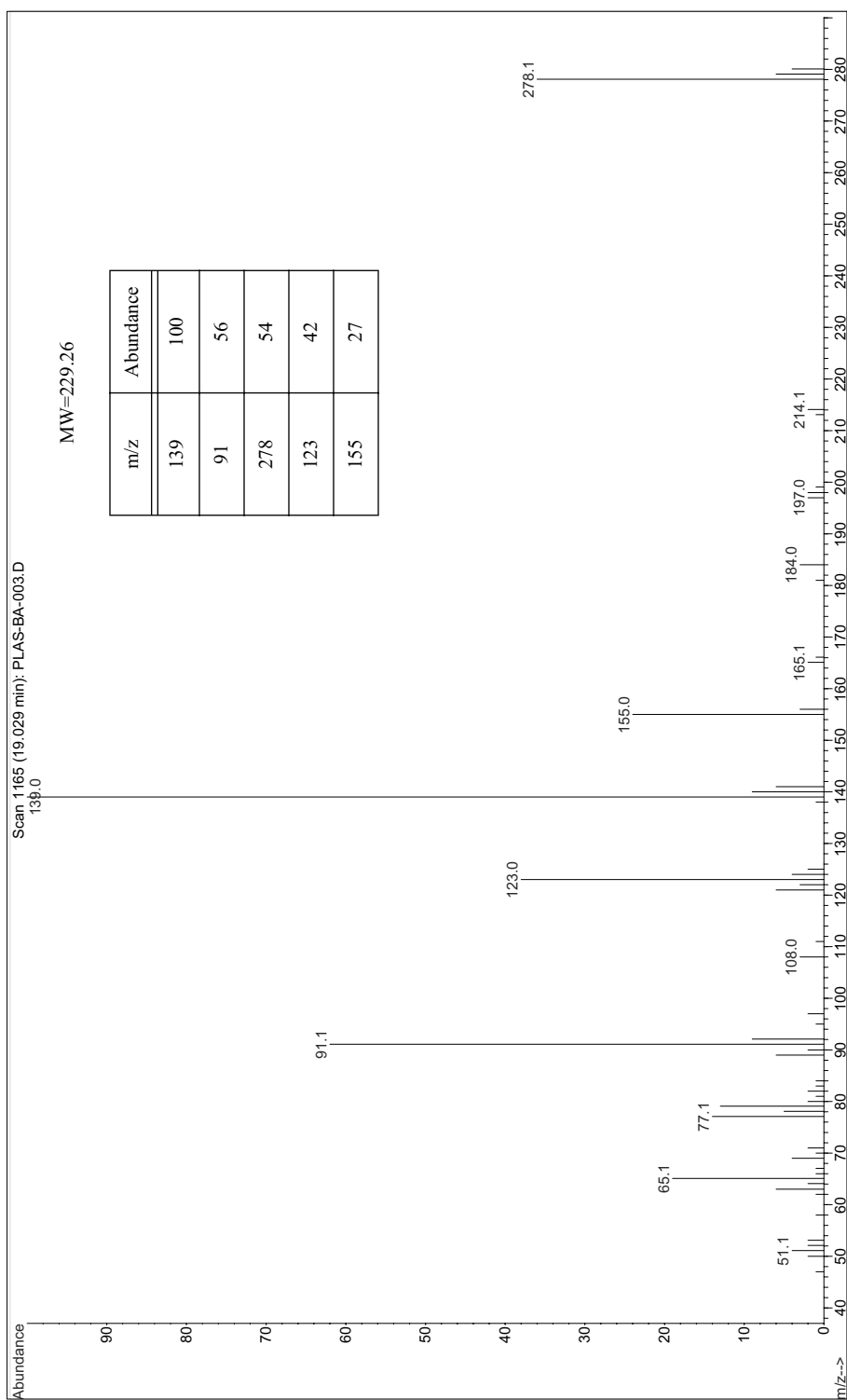
Contains no hazardous air pollutants or ozone depleting substances. It is also not listed under the US Clean Water Act Priority Pollutant List.

Point of Release

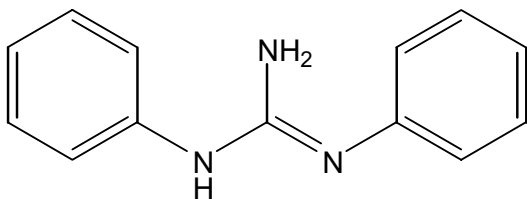
Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

No specific human health toxicity data is available for this product.

Mass Spectrum for Celogen® RA - PLAS-BA-003

For Chromatogram See Appendix A - PLAS-BA-003 - page 601

Perkacit® DPG

CAS Number 102-06-7
RTECS Number MF0875000
Abbreviation DPG

Formula C₁₃H₁₃N₃
Molecular Weight 211.27

Chemical Name

N,N'-diphenylguanidine

Synonyms

1,3-diphenylguanidine; diphenylguanidine; DPG; melaniline; sym-diphenylguanidine

Brand Names & Manufacturers

Vanax® DPG	R.T. Vanderbilt Company, Inc.
Vulkacit® D	Lanxess
Soxinol® D	Sumitomo Chemical Co., Ltd.

Physical Properties

Appearance	White to pale-yellow powder					
Melting Point	150 °C		Boiling Point Decomposes 170 °C			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water 0.08	MeOH U	EtOH 40-80	Acetone U	CH₂Cl₂ 40-80	Hexane U

Application, Regulatory & Environmental Information

Application Used as a secondary accelerator with thiazoles and sulfenamides in NR and SBR compounds. Exhibits better storage stability compared to thiuram and dithiocarbamates but is not as active. Perkacit® DPG can be used in latex as a foam stabilizer in the silico-fluoride foam process.

Regulatory Information

FDA approved for use as an accelerator in the manufacture of rubber material (up to 1.5% of weight of rubber) intended for use in all stages of production, processing, packaging, and transport of food under 21CFR177.2600.

Environmental Impact

Does not bioaccumulate or persist in environment: Biodegradability: > 90% in <2 weeks. Considered to be toxic to aquatic organisms.

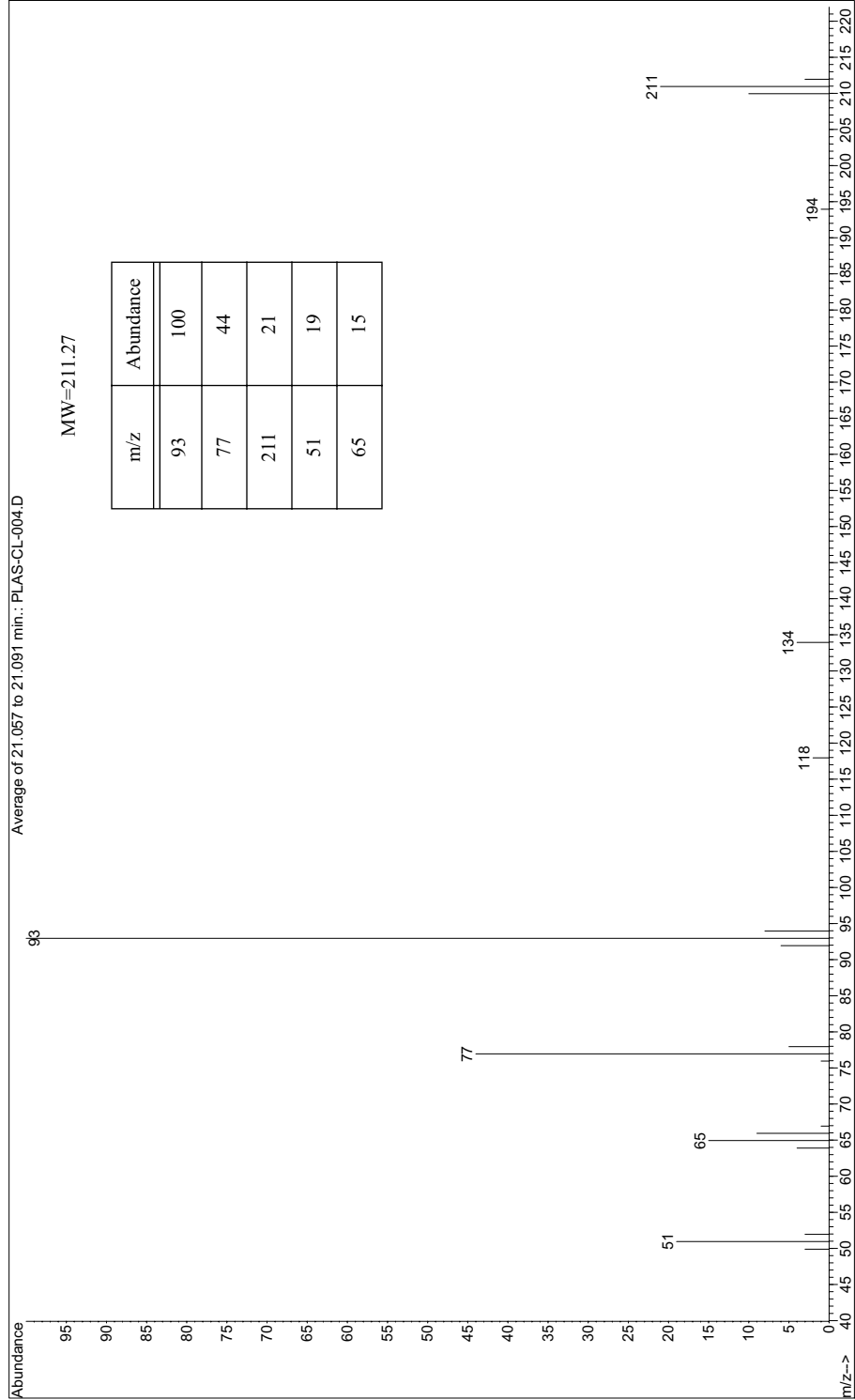
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Toxicity of this compound is considered low. Not carcinogenic, with negative to weak results in genotoxicity tests, but does cause reproductive/blood effects. Acute oral (LD50): 350–507 mg/kg [Rat], acute dermal (LD50): >2000 mg/kg [Rabbit].

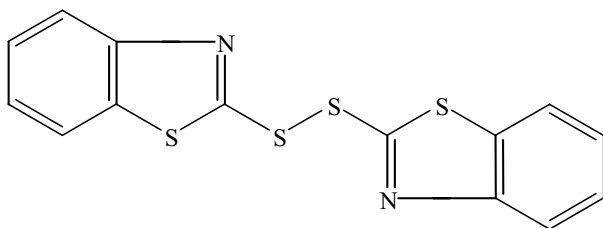
Mass Spectrum for Perkacit® DPG - PLAS-CL-004



For Chromatogram See Appendix A - PLAS-CL-004 - page 602

Perkacit® MBTS

Akzo Nobel Chemicals B.V.

**CAS Number** 120-78-5**RTECS Number** DL4550000**Abbreviation** DTBT**Formula** C₁₄H₈N₂S₄**Molecular Weight** 332.48**Chemical Name**

2,2'-dithiobis(benzothiazole)

Synonyms

benzothiazole disulfide; di-2-benzothiazolyl disulfide; dibenzoyl disulfide; 2,2'-dithiobisbenzothiazole; 2-mercaptobenzothiazole disulfide

Brand Names & Manufacturers

Altax® (MBTS)

R.T. Vanderbilt Company, Inc.

Naugex®

Chemtura Corporation

Thiofide

Solutia Inc.

Physical Properties**Appearance** Off-white powder**Melting Point** 177-180 °C**Boiling Point** 260 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
<0.1		40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information

Application Used as a medium-fast vulcanization accelerator for butyl, isoprene, and diene (natural and synthetic) rubbers. Also used as a retarder in neoprene. Commonly found in industrial rubber products such as footwear, hose, roofing, and automotive components.

Regulatory Information

FDA approved for use in articles in contact with food as specified under 21CFR177.2600 and 175.105.

Environmental Impact

Undergoes sunlight photolysis with T(1/2) of 3 hours, slightly susceptible to indirect photolysis. Product is considered harmful to aquatic organisms and has a low to moderate potential to bioaccumulate based on an estimated log Pow value of 4.2.

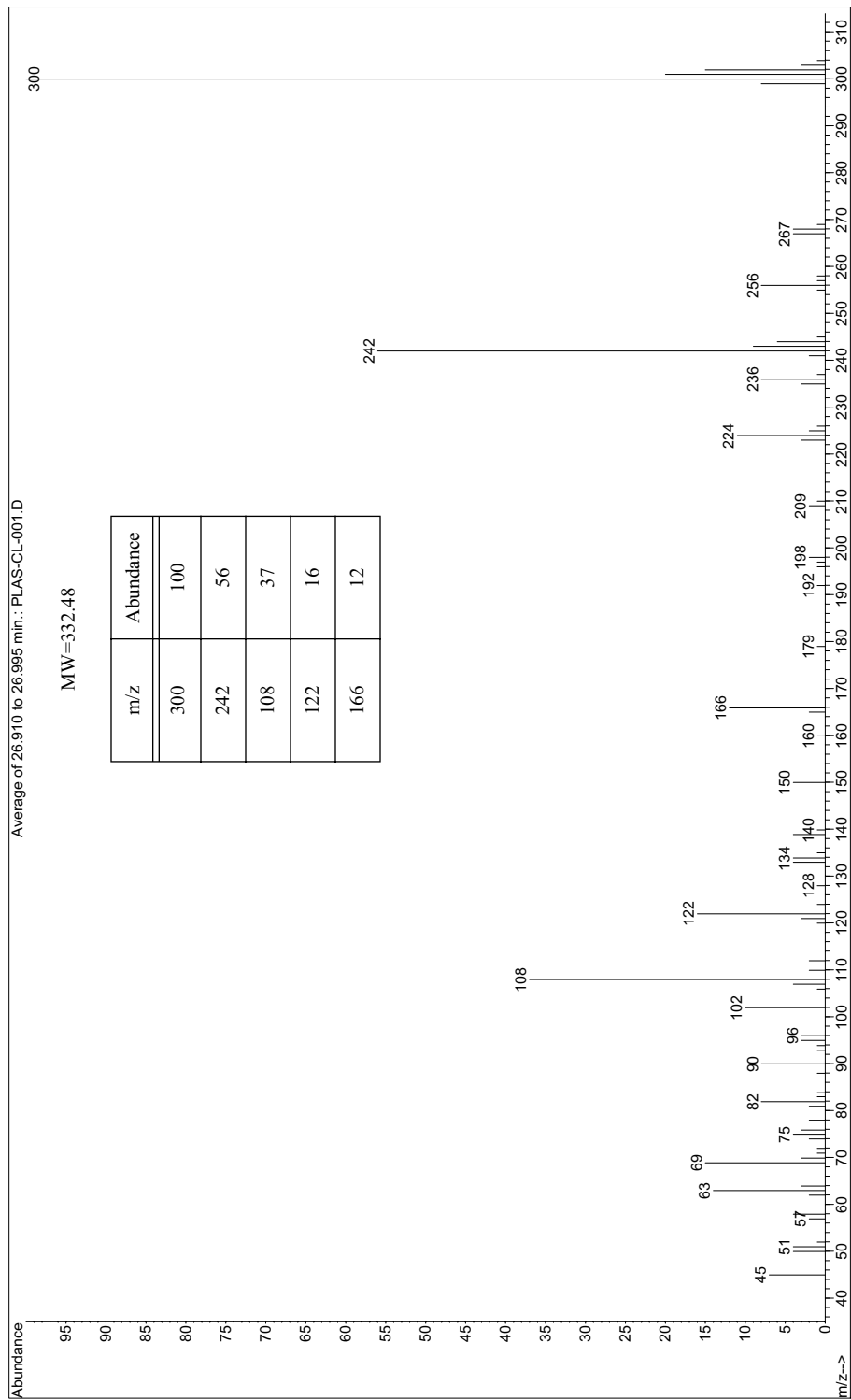
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Toxicity of DTBT is low. No evidence of carcinogenicity or gonadotoxicity. Only a minor dust hazard. Acute oral (LD50): >7940 mg/kg [Rat]; acute dermal (LD50): >7940 mg/kg [Rabbit].

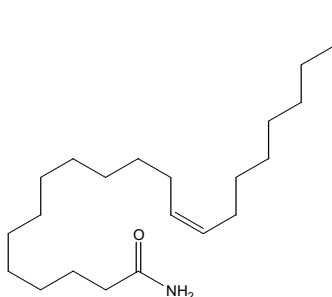
Mass Spectrum for Perkacit® MBTS - PLAS-CL-001



For Chromatogram See Appendix A - PLAS-CL-001 - page 603

Kemamide® E ultra

Chemtura Corporation

**CAS Number** 112-84-5**RTECS Number** N/A**Abbreviation** Not Identified**Formula** C₂₂H₄₃NO**Molecular Weight** 337.58**Chemical Name**

erucamide

Synonyms

erucyl amide; 13-docosenamide; (Z)-docos-13-enamide

Brand Names & Manufacturers

Kemamide E ultra

Chemtura Corporation

Physical Properties**Appearance** Powder**Melting Point** 80-85 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
<0.01	10	10	10	U	U	U

Application *Application, Regulatory & Environmental Information*

Additive used for thermoplastic applications requiring lubrication, slip, and anti-blocking properties. Commonly used in polyethylene and polypropylene films, as a lubricant in polyvinyl chloride, mold release agent, dyestuff dispersant for printing inks and surface coatings, and a blending agent for polyamide resins.

Regulatory Information

FDA approved for use with rubber food-contact materials per 21CFR178.2010 or 178.3860.

Environmental Impact

Not expected to be an immediate hazard to the environment. Long-term effects have not been thoroughly investigated.

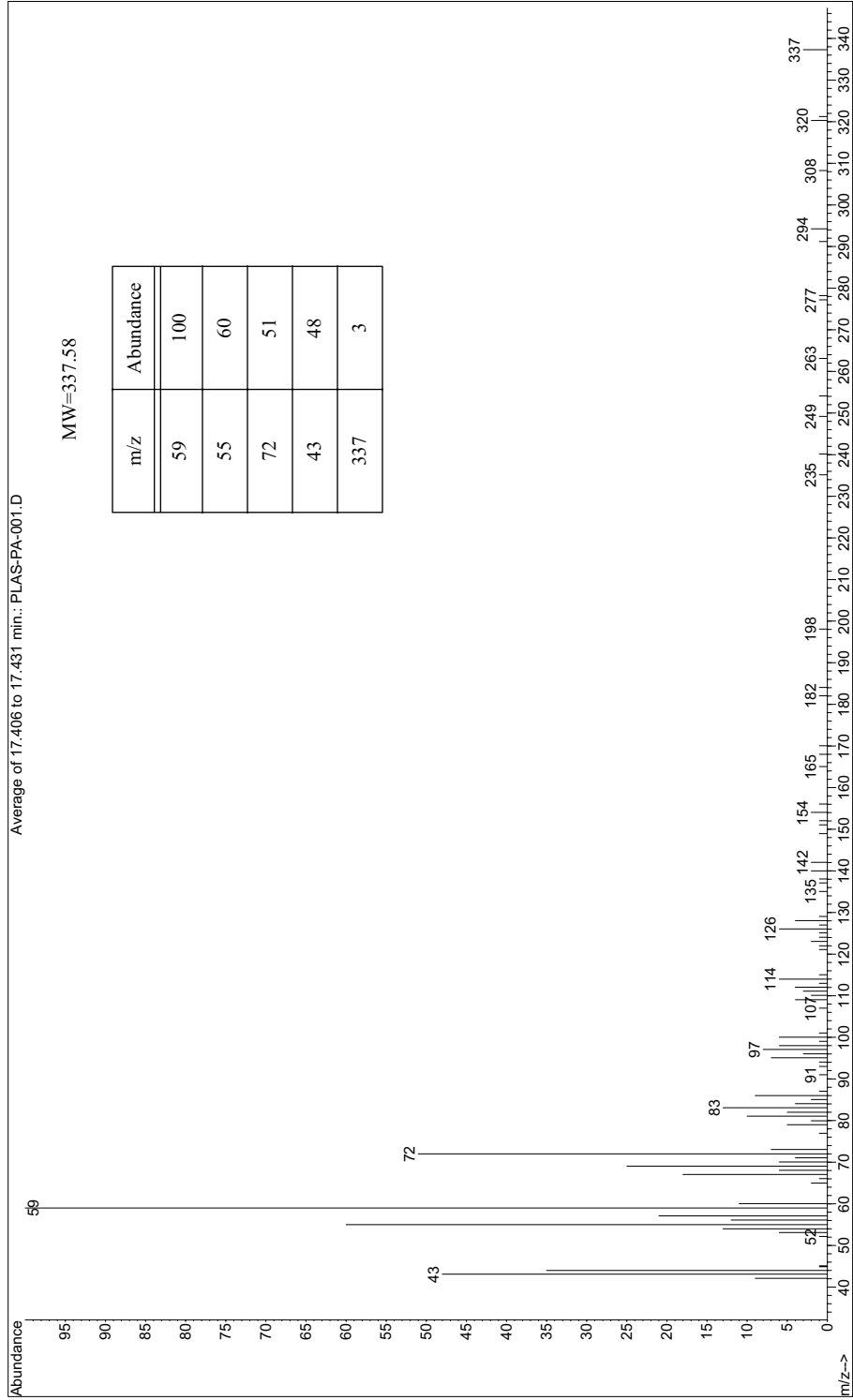
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA. Also not listed on California Proposition 65.

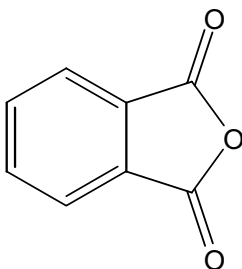
Mass Spectrum for Kemamide® E ultra - PLAS-PA-001



For Chromatogram See Appendix A - PLAS-PA-001 - page 604

Retarder AK

Akrochem Corporation

**CAS Number** 85-44-9**RTECS Number** TI3150000**Abbreviation** Not Identified**Formula** C₈H₄O₃**Molecular Weight** 148.12**Chemical Name**

phthalic anhydride

Synonyms

1,3-isobenzofurandione; phthalic acid anhydride; 1,2-benzenedicarboxylic acid anhydride

Brand Names & Manufacturers

Retarder AK

Akrochem Corporation

Physical Properties**Appearance** White powder**Melting Point** 123-132 °C**Boiling Point** 284 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	1-10	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information

Application Retarding agent for most types of rubber. Also used as an intermediate in the production of pigments and dyes, agricultural, pharmaceutical, and several other chemical products. Phthalic anhydride containing materials are used in coatings applications for home appliances, automobiles, medical devices, and furniture.

Regulatory Information

Regulated by the EPA under the Clean Air Act as a hazardous air pollutant and the Clean Water Act as a hazardous water pollutant. Phthalic anhydride is approved by the FDA for a variety of food contact applications.

Environmental Impact

When released to moist soil or water, this material is expected to hydrolyze. When released into water, this material is not expected to evaporate significantly, and it will have a half-life of less than 1 day. This material has an estimated bioconcentration factor (BCF) of less than 100. This material is not expected to significantly bioaccumulate. When released into the air, this material is expected to have a half-life of greater than 30 days.

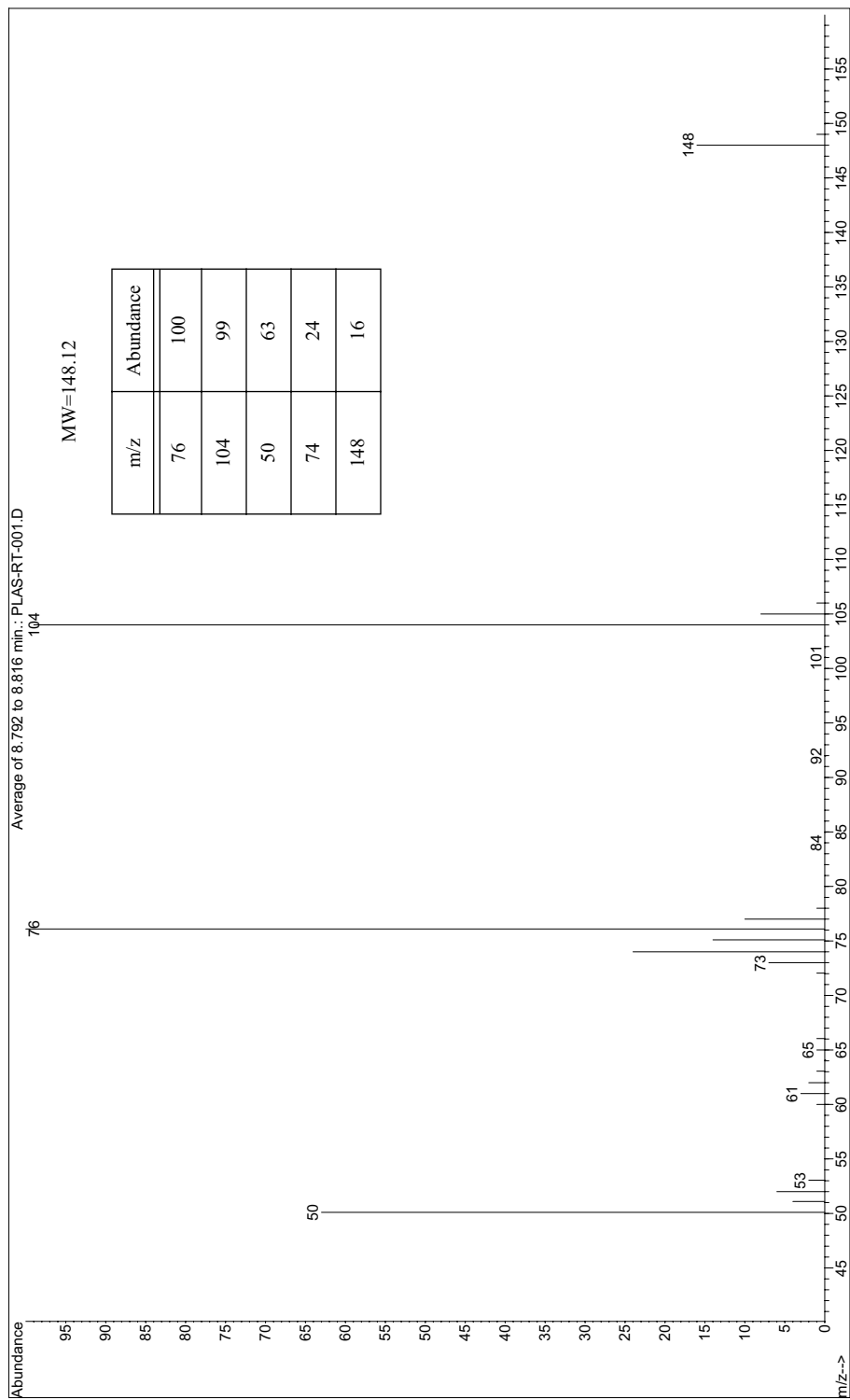
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, consumers may be exposed to phthalic anhydride from the use of plastics, furniture, glues, coatings, and home products from which phthalic anhydride may leach, and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): 1530 mg/kg [Rat], acute dermal (LD50): >10 gm/kg [Rabbit]. Acute inhalation (1 hour) (LC50): >210 mg/m³ [Rat]. Has shown teratogenic effects in laboratory animals. Not listed as a carcinogen by IARC, NTP, ACGIH, or OSHA.

Mass Spectrum for Retarder AK - PLAS-RT-001



For Chromatogram See Appendix A - PLAS-RT-001 - page 605

Stearic Acid RG (rubber grade)

Akrochem Corporation

CAS Number 57-11-4**RTECS Number** WI2800000**Abbreviation** Not Identified**Formula** C₁₈H₃₆O₂**Molecular Weight** 284.48**Chemical Name**

stearic acid

Synonyms

octadecanoic acid; cetylacetic acid; 1-heptadecanecarboxylic acid

Brand Names & ManufacturersGlycon[®] DP

Glycon Corporation

Physical Properties**Appearance** Colorless, waxy solid**Melting Point** 67-72 °C**Boiling Point** 361 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	U	40-80	U

Application *Application, Regulatory & Environmental Information*

Dispersing agent and accelerator activator in rubber compounds. It aids dispersion of pigments and fillers and improves processing since it acts as a stock lubricant and can facilitate mold flow, improve extrusions, and aid release.

Regulatory Information

FDA approval for food contact applications under 21CFR184-1090. On the FDA GRAS (generally approved as safe) list.

Environmental Impact

When released into soil or water, this material is expected to readily biodegrade.

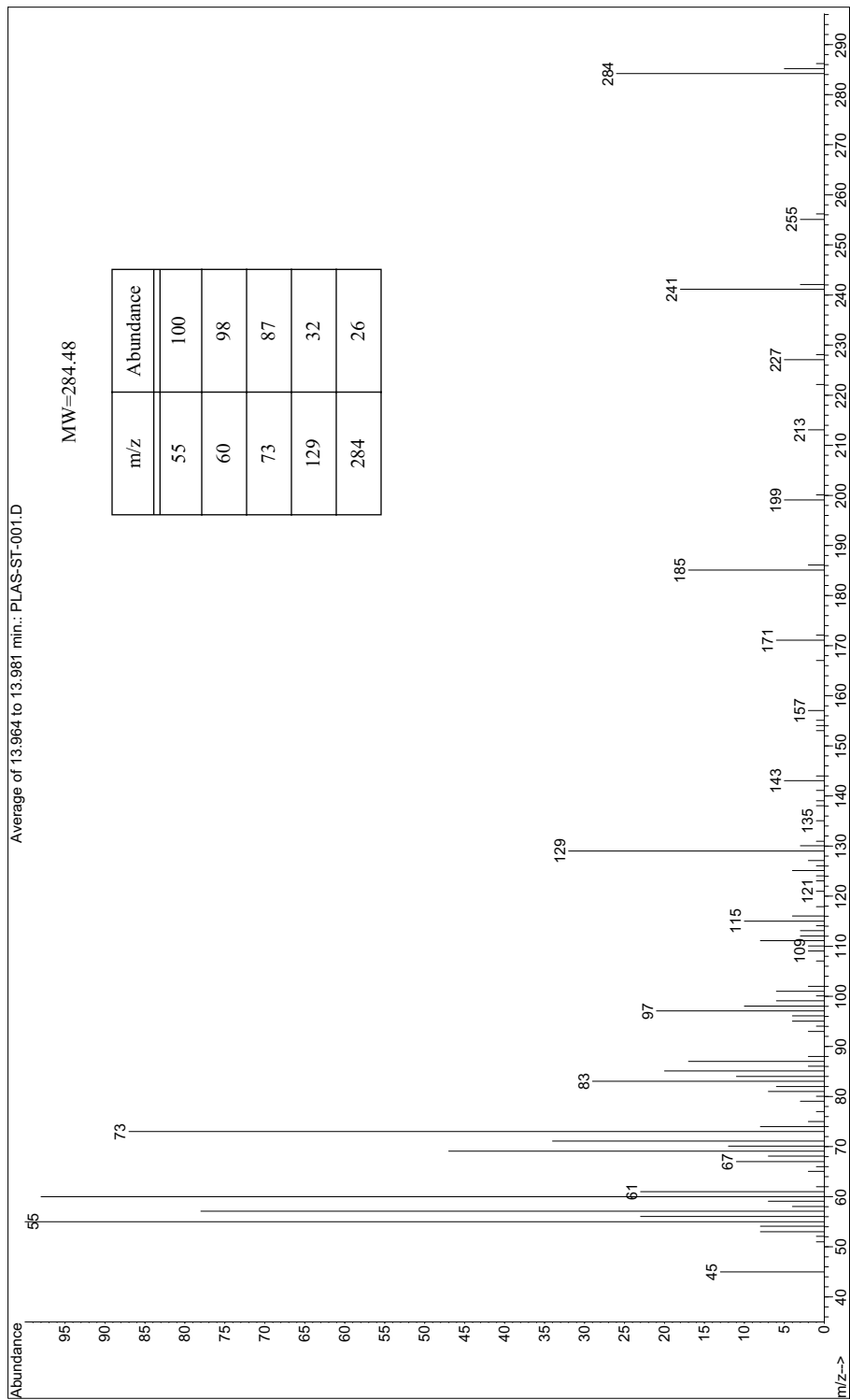
Point of Release

Can be released as point source pollution during manufacture, transportation, and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): >2000 mg/kg [Rat], acute dermal (LD50): >5000 mg/kg [Rabbit].

Mass Spectrum for Stearic Acid RG (rubber grade) - PLAS-ST-001



For Chromatogram See Appendix A - PLAS-ST-001 - page 606

Practical Applications of Investigative Analyses

Introduction

Chemical analysis of polymeric compounds may be undertaken for many reasons, including troubleshooting, review for specific applications, compositional verification, regulatory compliance, fundamental development, and other reasons. It is from such applications that the concept of this Handbook originated. Culled from the archives of two of the authors of this book (Groeger and Hubball) are some interesting and illustrative case studies. Each is presented with background on the corresponding issues.

CASE STUDIES: POLYMER ADDITIVES IN PHARMACEUTICAL PACKAGING

Background

Packaging for active pharmaceutical compounds ranges from simple tablet bottles, vials, and blister packs, to complex respiratory delivery devices that combine dry powder dispersions with a controlled airflow for asthma therapy. Other devices include point-of-delivery mixing of drug ingredients, pumps, diffusion membranes, and more. These may include polymer-coated metals, polymeric packaging with internal metal components, and combinations of thermoplastics, elastomers, and/or metals. Some polymers are infused with a drug compound designed to desorb in transdermal or transocular diffusion-based systems. Technical packaging components are engineered to achieve uniform drug stability and controlled dose delivery rate in a patient-ready form.

Although some packaging suppliers perform development work, many drug delivery systems are designed by pharmaceutical companies. This is especially true when a new device is required for which there is no precedent. Packaging suppliers also perform original development work in collaboration with pharmaceutical manufacturers. In some cases, existing devices are modified. A barrier/release coating for the interior surface of an aluminum alloy metered dose inhaler (MDI) canister might be developed by a pharmaceutical manufacturer, for example. Implementation of the design is then taken to a manufacturer for commercial production, during which time tooling is developed for the components or processes. Engineers or technologists typically select materials based on engineering properties. Impact resistant ABS (acrylonitrile-butadiene styrene polymer) might be selected for a particular component. A critical omission may be that the details of the formulation are not investigated at the outset. This might include, for example, the regulatory suitability of an antioxidant in the base polymer.

Additionally, subsequent analysis of the materials for compliance to various regulations is often based on routine solvent extraction protocols followed by GC/FID (flame ionization detector) analysis. These protocols are generally based on specific target compounds that are regulated rather than analysis for all compounds present. From our experience we have documented many problems related to such an approach. The following case studies emphasize the need for thoroughly analyzing materials for suitability early on in the developmental process.

Case Study #1: Pre-Filled Syringe Vials

Injectable pharmaceutical compounds are often pre-packaged into vials that are inserted into syringe barrels for patient delivery. In some cases, the vials contain contaminants. In the present example, the active compound inside this vial was sampled and found to contain acetophenone, dibutyl phthalate, stearic acid, and myristic acid, none of which are components of the drug

formulation. These substances each have negative health implications and are regulated for various applications.

Investigation into the vial manufacturing process was initiated to determine the root cause of the contamination. The vials are most commonly glass, since this provides an inert contact surface and transparency for inspection and dose verification. The vials must be sealed, and at one end a piston must be provided while at the opposite end a septum is fitted to allow puncture by the needle inside the syringe barrel. The elastomeric components of both are shown in Figure 10-1 and Figure 10-2. An aluminum ferrule that is crimped to form a seal after the vial is filled surrounds the diaphragm.



Figure 10-1 Crimped Diaphragm on Pre-Filled Syringe Vial

The pharmaceutical formulation inside this vial was subjected to GC/MS analysis at the end of its shelf life and the contaminants were identified. GC/MS analyses of the vial piston and diaphragm materials were also conducted. Analysis of the vial piston shows a range of nitrile fragments, consistent with nitrile rubber. Silicone is typically present on this type of component to provide lubricity inside the bore of the glass vial. Acetophenone was also found. This is a thermal decomposition product from the peroxide crosslinking agent in the rubber (dicumyl peroxide). Stearic and myristic fatty acids were present and are typically added in the manufacturing process during mixing to reduce shear viscosity. These materials leach into the pharmaceutical compound over time. The result is that regulated, non-formulation organic compounds are inadvertently injected in unknown concentration directly into the bloodstream of the patient who may already have compromised health.

The root cause of this problem goes beyond determining and stopping the source of the contaminants. The root cause of the problem was that the designers of the vial did not consider contamination during the original design. The corrective action was to change the design approach such that chemical analysis of all raw and manufactured materials would be implemented during



Figure 10-2 Piston on Pre-Filled Syringe Vial

the development process. Increased oversight of the supplier network followed, as well as significantly tightened specifications.

Case Study #2: Nasal Pump Delivery System

A wide range of over-the-counter and prescription pharmaceutical products use manually actuated pumps. A common example is the nasal pump spray container. When the design of these pumps allows contaminated products to be used, the patients and the manufacturer have a problem. This was the case, when palmitic, myristic, stearic, and oleic fatty acids (all non-formulation ingredients) were found in a nasal spray product.

The investigation was begun after patient complaints that the pumps became blocked over time. Pumps typically deliver a low pressure, fine droplet-sized mist at a controlled dose rate. Proper control of the dose rate and spray pattern requires precision molding and assembly of the package components and consistent performance of these components when they are in contact with the drug product for extended periods, over a wide temperature range. These components are made of

thermoplastic, elastomeric, and metallic materials. The pump actuator and its internal elastomeric check valve are vital components. The design is shown in Figure 10-3.

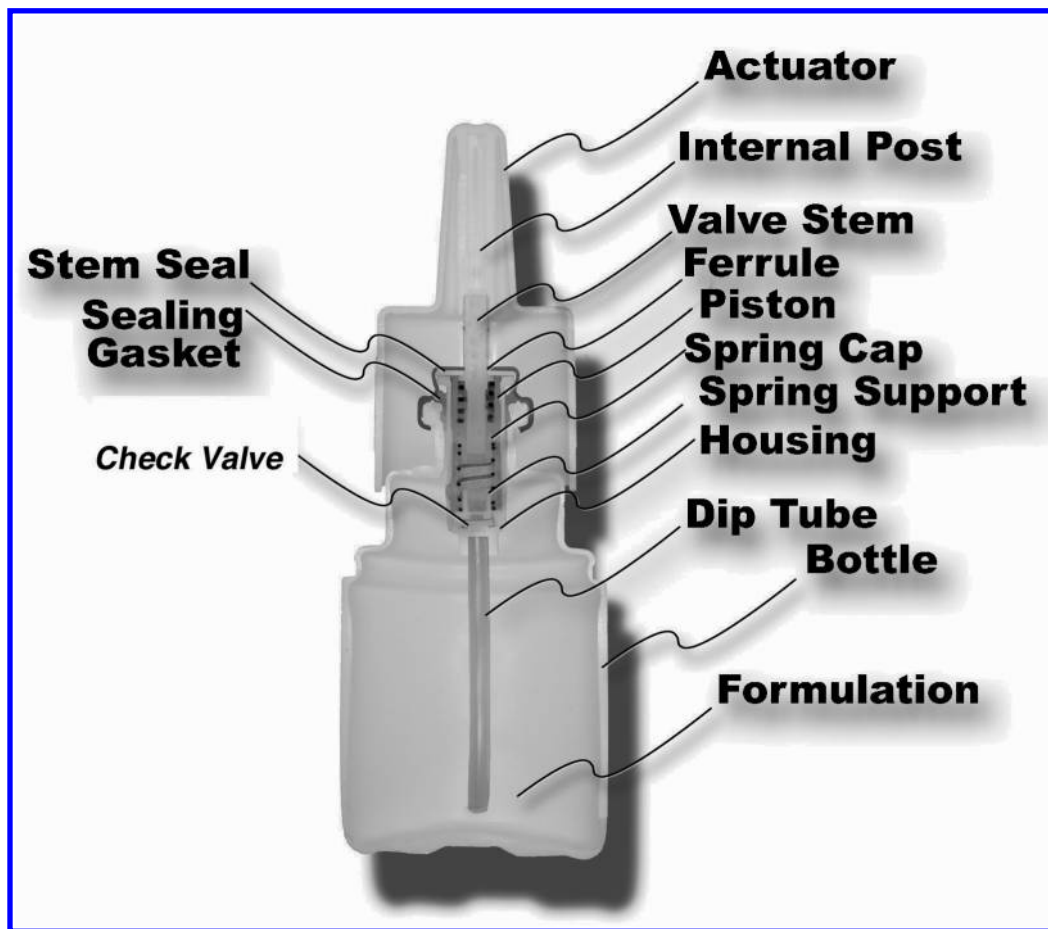


Figure 10-3 Nasal Pump Design

The drug formulation contains an active ingredient, a thixotropic adjunct to promote drug retention on mucosal surfaces, water, stabilizers, a buffer, and alcohol.

In the course of the investigation into the blockage of the nasal spray actuators, devices that passed 100% spray-testing at the time of manufacture were found to become blocked after an extended period of non-use. Investigation into the blockage revealed nothing unusual about the drug formulation. When a new actuator was placed on the pump, normal action resumed. Blockage within the actuator was removed and analyzed by GC/MS and was found to contain formulation ingredients plus fatty acids. These included palmitic, myristic, stearic, and oleic fatty acids. A gelled substance was present on the elastomeric check valve. This gelled substance is shown in [Figure 10-4](#).

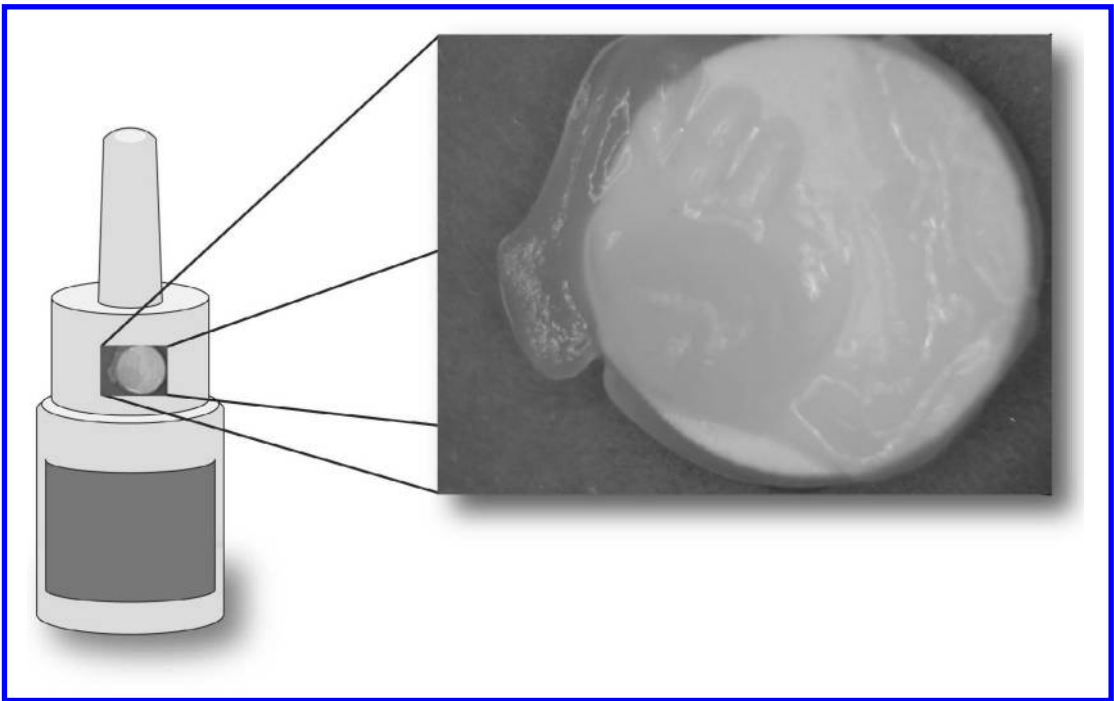


Figure 10-4 Gelled Nasal Formulation on Elastomeric Check Valve

The investigation turned to identification of the gelled substance. Analyses indicated that fatty acids were included in the rubber formulation for the actuator gaskets. Laboratory experiments then replicated the formation of the gelled substance through interaction between the double bonds of the oleic acid and one of the formulation ingredients. The drug formulation is often in stagnant contact with this elastomeric seal and that caused the gelled material to form on the actuator surface. At some point, the gelled material would break away. The high viscosity of the gel would not allow it to pass through the narrow internal passages inside of the actuator. [Figure 10-5](#) presents the GC/MS analysis summary. The other compound found, the alkyl phenol, is an antioxidant. Specific identification of these compounds was made possible through comparison of mass spectra with reference materials.

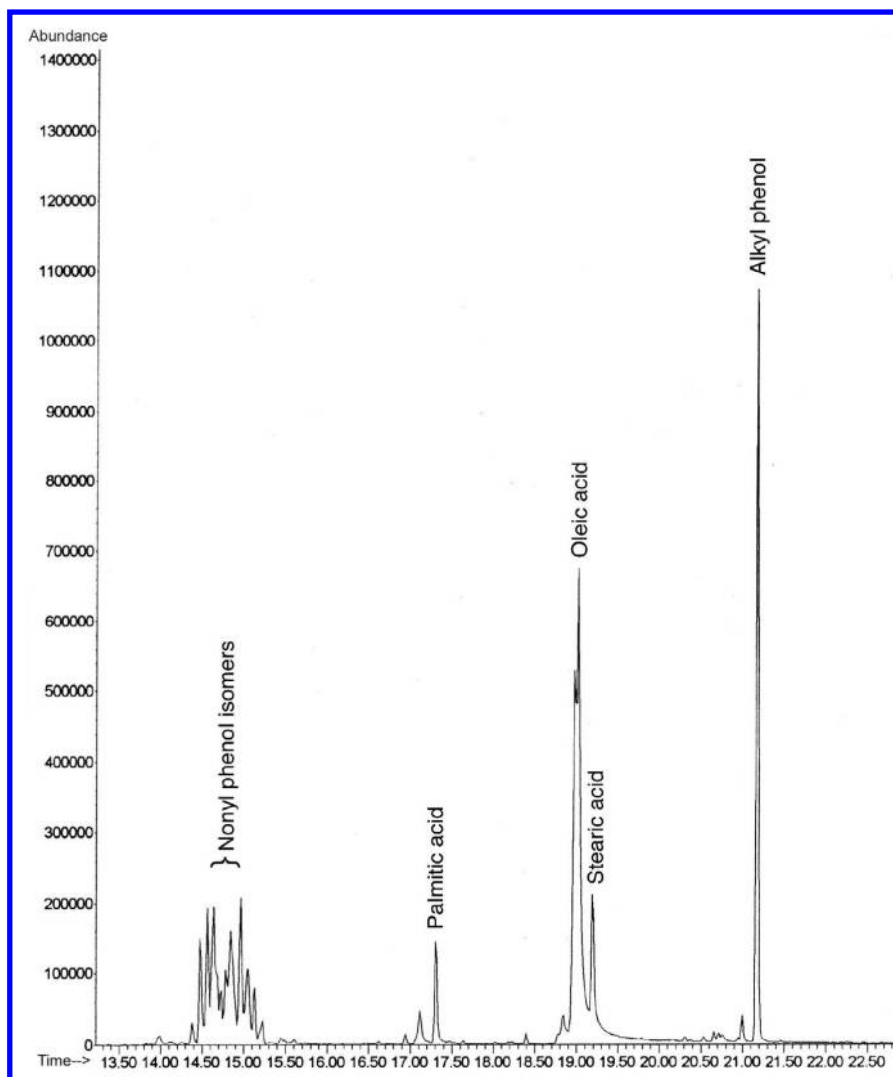


Figure 10-5 GC/MS Chromatogram of Ethanol Extract of Elastomeric Gasket

The original problem had been identified as a clogged pump. However, in the course of the investigation, it became apparent that contaminants had entered the drug formulation due to interaction between the drug and the container material. Corrective actions included reformulation of the elastomeric materials in the container and increased controls on all packaging materials. In addition to the requisite routine analytical reviews of the pharmaceutical ingredients and package, investigative analyses using GC/MS were implemented.

Case Study #3: Dry Powder Inhalation Device

Dry powder inhalers have been in the market for approximately 20 years. Their use is increasing due to new forms of medications that can be microencapsulated in a manner that permits deep pulmonary delivery. As all products intended for human use must be considered for possible contaminants, it was surprising that in one recent case, dry powder inhalers were found to contain many compounds not found in the original formulation, including phthalates, alkanes, branched chain hydrocarbons, and alcohols. Investigation of the root cause for contamination demonstrates that not only the materials of the container need to be reviewed, but also the processing of those materials.

For one such device, polycarbonate was chosen from a particular supplier to form a high strength component that directly contacts the drug delivery stream. During chemical testing of devices from several Production Qualification (PQ) lots, anomalous analytical results were obtained with GC/MS sampling of the polycarbonate component. [Figure 10-6](#) presents the analysis of the initial, qualified polycarbonate compound analyzed by thermal desorption GC/MS. This analysis contains traces of thermal decomposition products of the polycarbonate, an antioxidant, and a trace of bisphenol A (BPA), one of the starting materials for polymerization of polycarbonate. A commercial compounder prepared this polycarbonate with a specific non-staining antioxidant that is safe for drug contact. While BPA would not be desirable for patient contact, this compound was accepted, as it was believed that this trace concentration could not reach the patient through normal use of this device.

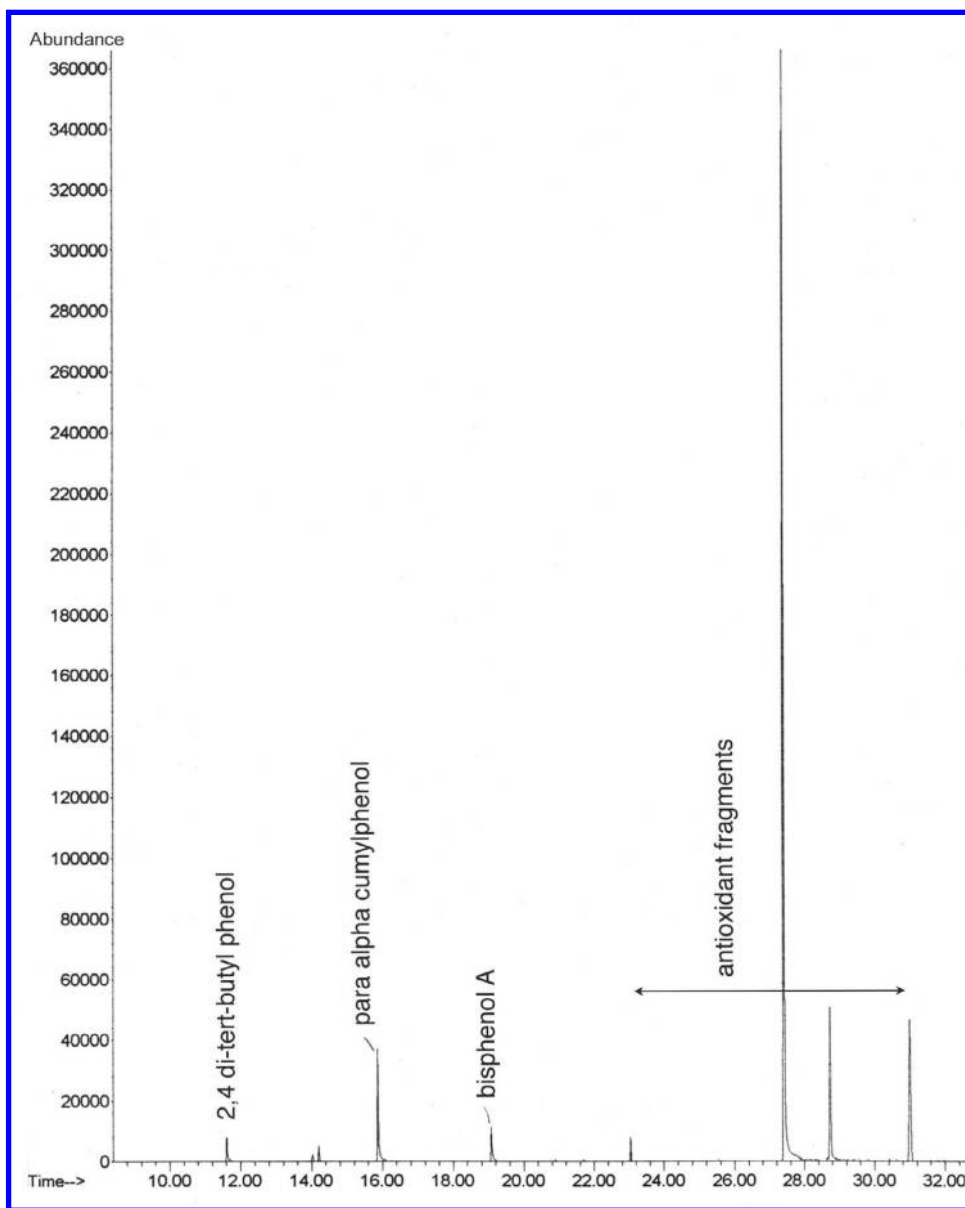


Figure 10-6 GC/MS Chromatogram of Polycarbonate Part of Dry Powder Inhaler

While subjecting two other PQ lots of these components to GC/MS analysis, the polycarbonate formulations were found to be very different from the original. [Figure 10-7](#) shows the analysis of a second PQ run and [Figure 10-8](#) shows a third PQ run. The second and third PQ lots were found to contain many compounds not found in the original, including phthalates, alkanes, branched chain hydrocarbons, and alcohols. The third run also contained fatty acids. This level of inconsistency led to a production hold on this device and subsequent investigation.

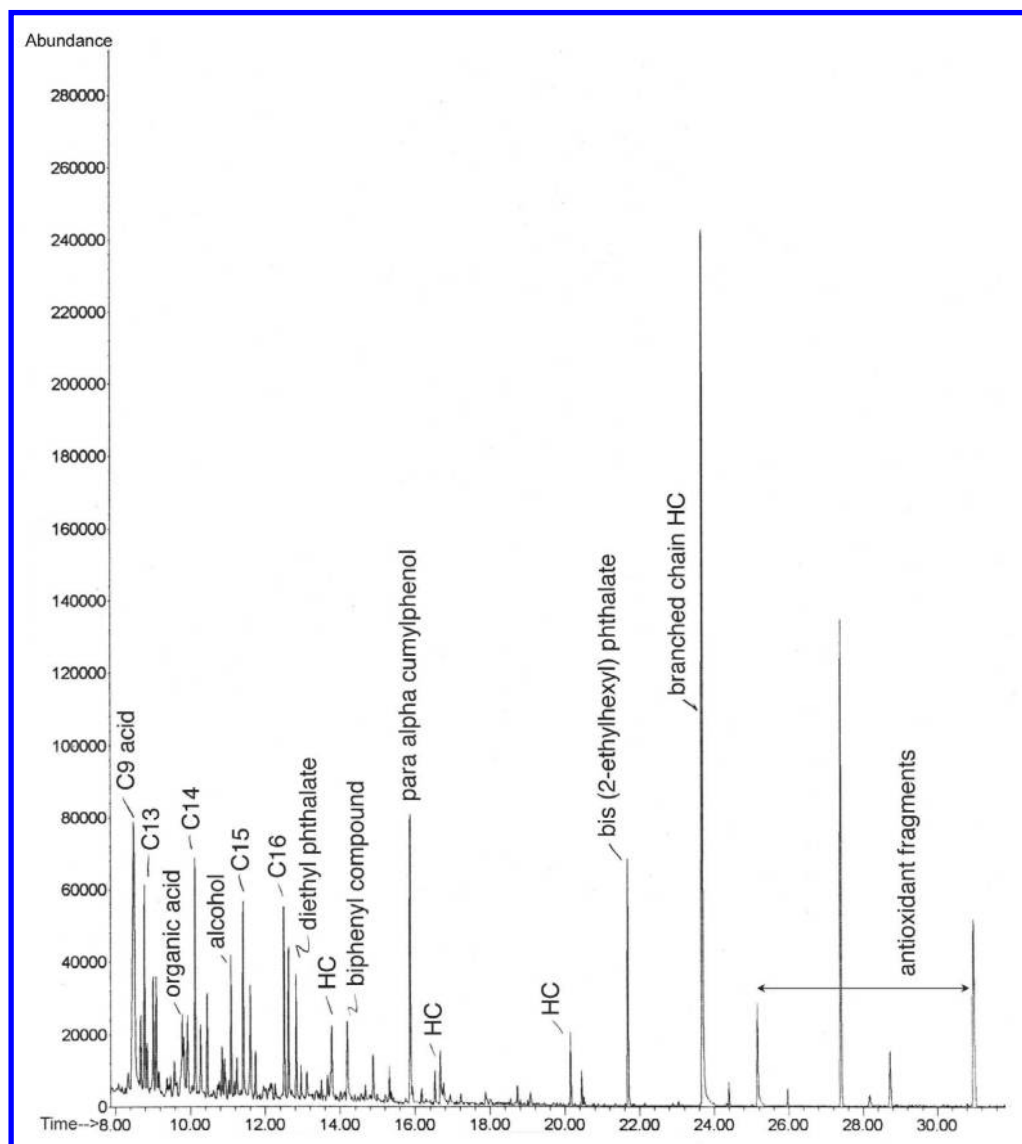


Figure 10-7 GC/MS Chromatogram of Polycarbonate Part of Dry Powder Inhaler, Second Lot

The supplier of the base polycarbonate resin provided all production details and controls, and site visits confirmed that it was highly unlikely that the base resins could vary in this manner. The commercial compounding site was visited and production runs of this and other resins were witnessed and reviewed. It was discovered that the mixing equipment was being shared and was used for mixing other polymers from other customers. Adequate purging protocols were not in place to ensure that the material from previous runs was fully purged from the mixing system before the next run was started. Corrective actions included amending the processing work instructions and training to include more complete purging methods. The manufacturer of the dry powder inhalation device also amended its own formulation specifications to include review of the purging methods.

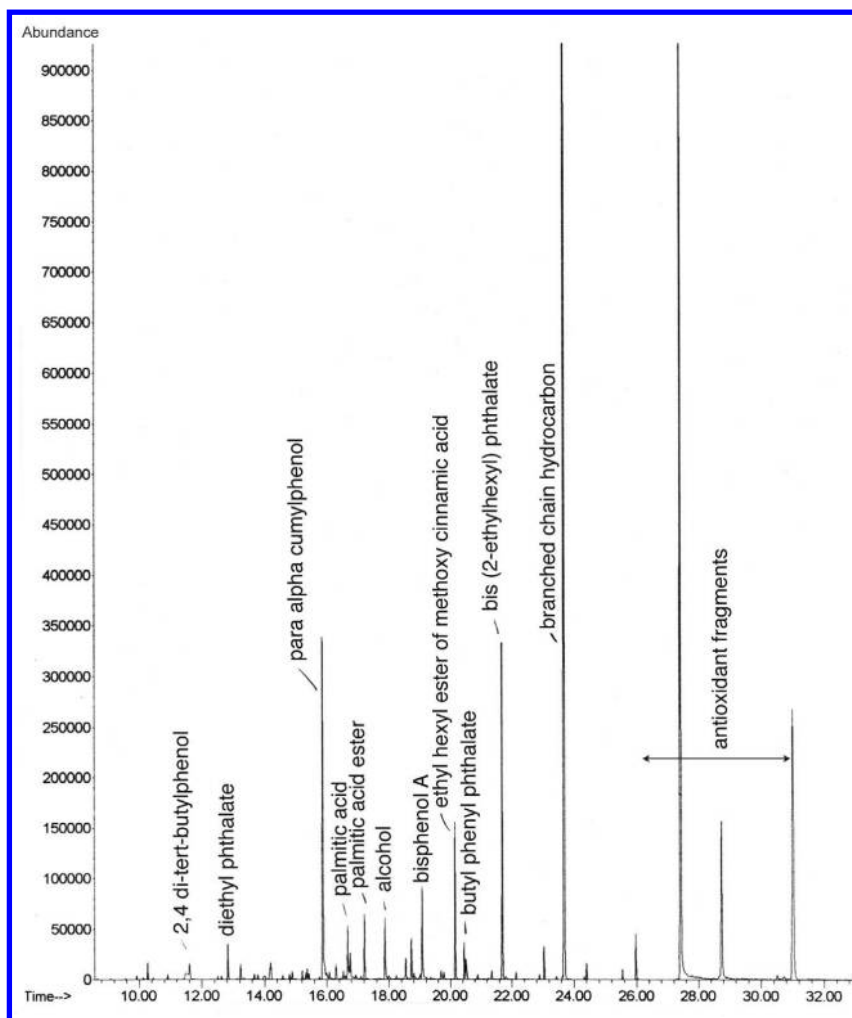


Figure 10-8 GC/MS Chromatogram of Polycarbonate Part of Dry Powder Inhaler, Third Lot

CASE STUDIES: PERFORMANCE AND EXPOSURE ISSUES WITH ORGANIC ADDITIVES

Introduction

Polymeric packaging materials come into contact with both finished goods and raw materials. Governmental agencies such as the US Food and Drug Administration (FDA) and agencies of the EU have regulations in place to monitor and control the presence and concentration of controlled substances in food and drugs. Packaging for other applications are largely unregulated. The three case studies that follow are examples of unintended contaminants that were discovered by analysis in packaged products.

Uses of Additives

Packaging manufacturers and their suppliers develop materials that must meet a wide range of requirements including cost competitiveness. Most packaging materials are commodity products, identified by a generalized description; therefore, the end product components are not strictly controlled. Common types of plastic packaging materials include low density polyethylene (LDPE), high density polyethylene (HDPE), polypropylene, polyethylene terephthalate (PETE), styrene, and many others. Typical minimum functional requirements for packaging include the following: tear resistance, acceptable appearance (transparency, translucency, color, or opacity), anti-blocking performance (plastic bags must open freely without sticking), integrity (no pinholes or gaps in seams), gauge, and type of material. It is rarely practical to identify a packaging material that contains only the requested polymer (without additives).

Formulations from any given supplier can be expected to change periodically, since the packaging manufacturer may source from a number of different resin and additive suppliers. This network is illustrated in [Figure 10-9](#). As indicated, the packager rarely has a direct relationship with the raw material suppliers; hence, there is no direct control over the packaging material formulations. Information provided in Material Safety Data Sheets (MSDS) is insufficient for controlling packaging for critical applications. The formulation details disclosed in this document address principal ingredients and do not contain details regarding specific compounds or master batch ingredients.

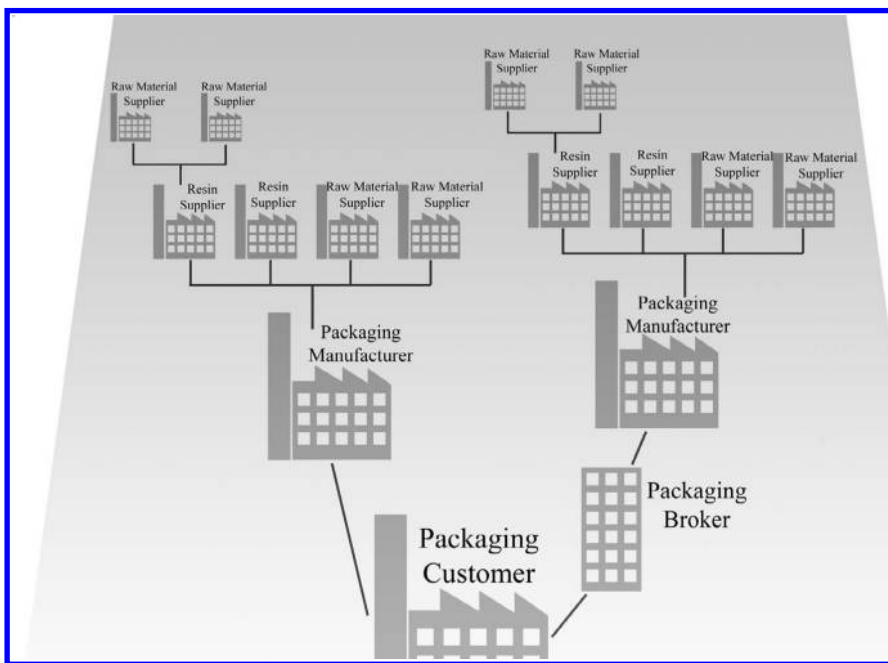


Figure 10-9 Packaging Supply Network

The type of process used also indicates the addition of polymer modifiers. Blow-molding requires that the polymer flows easily, while retaining good cohesive strength when molten to avoid introducing tears or voids. Melt flow modifiers are typically used for this purpose and include fatty acid esters, oleoamides, and adipates. Compounds of this type often also serve to prevent blocking (adhesion of one side of a bag to the other, for example).

Typical minimum requirements for the packaging necessitate the addition of other polymer modifiers. Prevention of discoloration requires addition of an antioxidant. The resin supplier is typically required to meet a general performance specification; however, the final use of the packaging may not be stipulated or considered when an antioxidant is chosen. Ultraviolet resistance is required for some packaging where extended sunlight exposure is expected. A common UV-inhibiting additive is carbon black.

Case Study #1: Contaminants in Plastic Food Packaging

Routine chemical analysis of a frozen food product containing unsaturated vegetable oils showed sporadic contamination with phthalates and erucamide, a fatty acid amide. Both substances are listed in the US FDA list of Indirect Food Additives as well as other regulations, and their presence in food is regulated. The subject food product was packaged in a heat-sealed polyethylene bag. The packaging supplier attributed the presence of these organic compounds on the surface of the frozen food product to sources other than their packaging; however, the packaging supplier stated that all of their film resin was sourced from a single supplier. The specification for this resin stipulated a melt flow index, a whiteness index for the pigment, tensile strength, elongation limit, and low density polyethylene as the base resin. [Figure 10-10](#) shows the composition of a typical package from this supplier. Thermal desorption GC/MS was applied and indicated hydrocarbons consistent with polyethylene plus butylated hydroxytoluene (BHT) as an antioxidant. BHT is approved as an antioxidant for food contact applications.

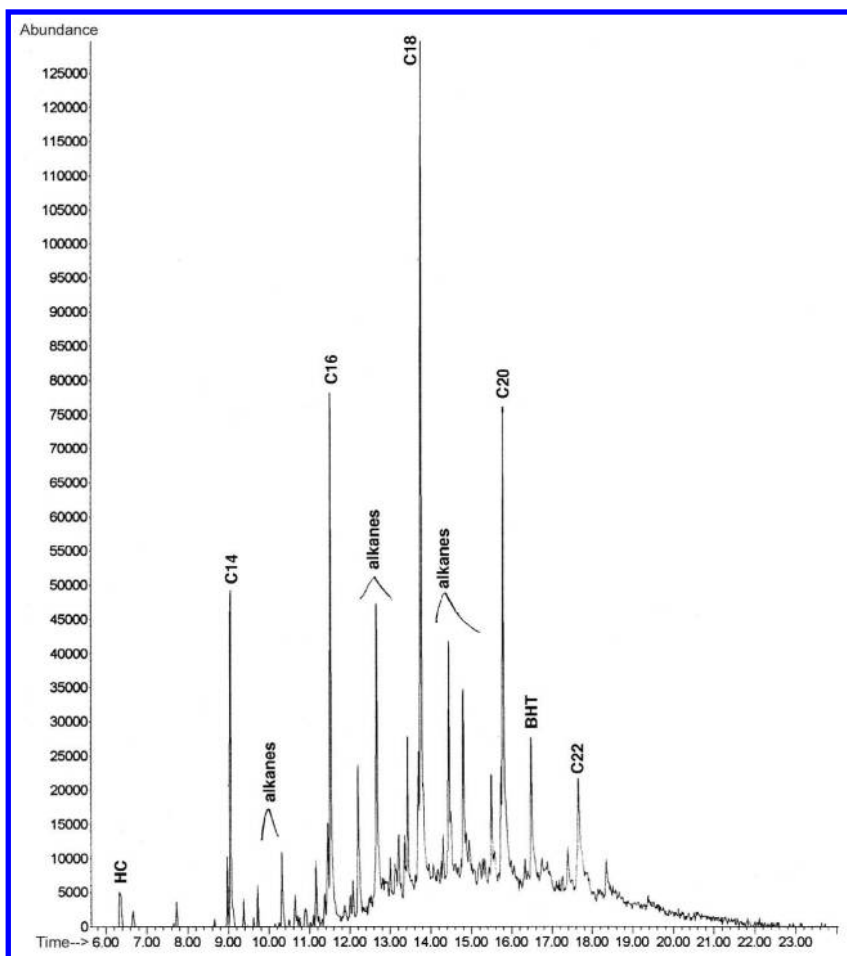


Figure 10-10 GC/MS Chromatogram of Typical Packaging Material

Investigation into the packaging film manufacturing processes was initiated. Incoming packaging materials were screened at the food production warehouse. The screening was based on appearance and feel as an initial basis. Packaging film with a distinctly waxy surface was identified as abnormal and analyzed by thermal desorption GC/MS. [Figure 10-11](#) shows the GC/MS analysis summary of one anomalous material sample indicating isobutyl phthalate, dioctyl phthalate, and erucamide as ingredients in the polyethylene film. These substances are named in the US FDA list of Indirect Food Additives and their presence in food is regulated. This anomalous packaging material was determined to be the cause of the food contamination.

Research into the source of these unexpected compounds determined that the packaging supplier had made a formulation change to offset the stiffness of a newer and less expensive source of polyethylene. The root cause goes beyond the source of the contaminants. It extends to why the formulation change was made without regard to the end use of the product. The corrective action

was for the supplier to more tightly control processes and to verify component changes with the customer.

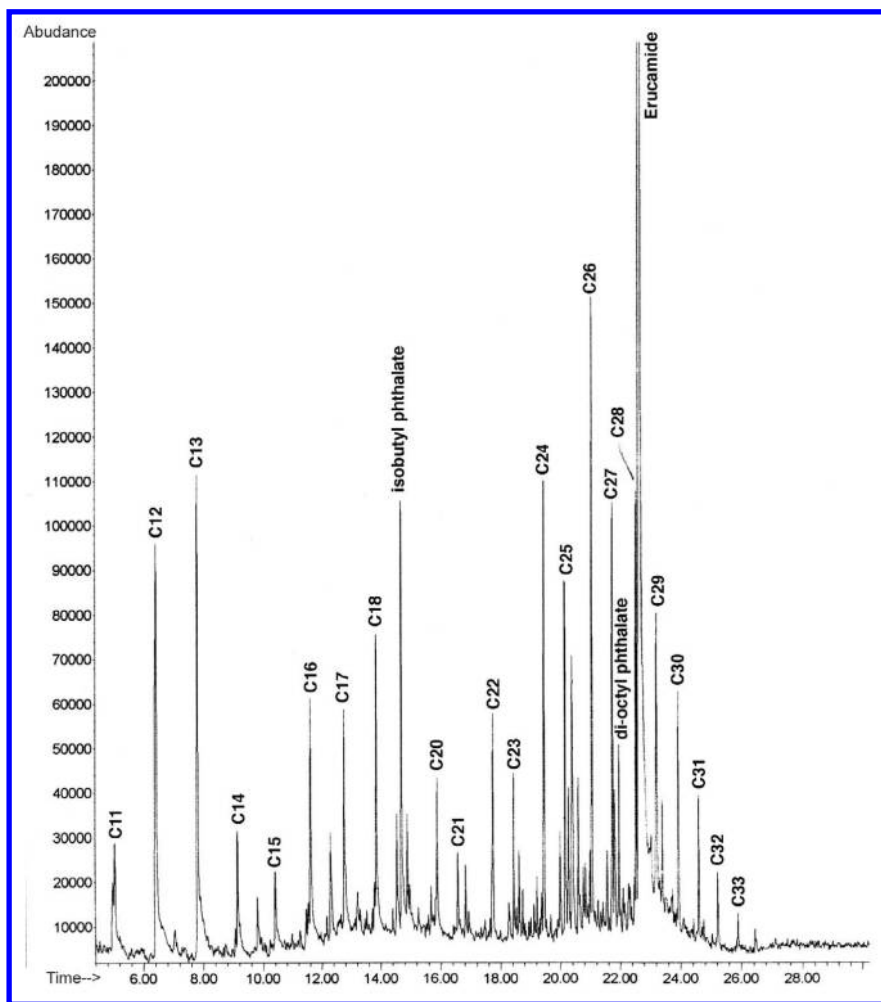


Figure 10-11 GC/MS Chromatogram of Anomalous Packaging Material

Case Study #2: Peeling Labels

Adhesive labels are used on many products and need to remain on the product for many reasons including safety, identification, and proper use of the product. In this case, the label adhesive failed and prevented further use of the equipment in which the product was used.

Batteries are typically produced with deep drawn metal cans on which a pressure sensitive adhesive label is affixed for product identification, branding, and safety information. Customers began complaining of batteries becoming jammed in various types of equipment. Devices returned to the manufacturer showed that the pressure sensitive labels had peeled back, resulting in adhesion between the overturned label and the device. Further examination of batteries that had been sitting on store shelves for more than a year also indicated peeling labels in a low frequency of batteries. These labels consisted of laminates of paper and polyester. The labels are normally flat and stiff

and when applied over a battery, the labels will return to the flat conformation if the adhesive fails. This results in peel-back at the edges of the label.

Investigation into the battery processing was initiated. Comparative GC/MS analysis of peeling and non-peeling areas of the labels indicated that the peeling areas contained phthalates and palmitic acid. Both perform as plasticizers in the pressure-sensitive adhesive used for these labels. Since the labels are printed in a continuous process, it was unlikely that only specific areas would be affected. This was consistent with the observed low frequency of label peeling, and eliminated the deposition of adhesive as a potential root cause.

The cans used to produce the batteries are deep drawn with a water-based lubricant that does not contain the phthalates or the palmitic acid. The cans are then washed in a phosphate surfactant and dried at high temperature. The cans are then bulk-packaged into cardboard gaylords, lined with plastic bags. In this case, the cans were dropped from the drying oven into the shipping container while still warm. Cans removed from the bag and randomly sampled by GC/MS showed no trace of phthalates or palmitic acid. However, upon further investigation, those cans that came into direct contact with the packaging were found with phthalates and palmitic acid on their surfaces. Results of the GC/MS analysis of the corresponding bag are shown in [Figure 10-12](#). This indicates that the bag contains diethyl phthalate, dibutyl phthalate, and palmitic acid. The phthalates serve as plasticizers for the bag and palmitic acid is a lubricant that blooms to the surface and renders the bag easy to open. Both features are completely inconsistent with the requirement to maintain the battery cans in a clean, contaminant-free condition.

Again, the root cause of the non-conformance was that the environment (in this case, the gaylords lined with the plastic bags) was not kept contaminant free. The more familiar connotation of “contaminant” by the labor force came in the form of particulates, wood fibers, cardboard fibers, insects, etc. At the Quality Control level, there was a lack of awareness about what constitutes a contaminant on the part of the can manufacturer. The corrective action was to educate the manufacturer about possible contamination, to review the manufacturer's processes, and to promote dialog between the manufacturer and the customer on matters affecting contamination, including processing and raw materials changes.

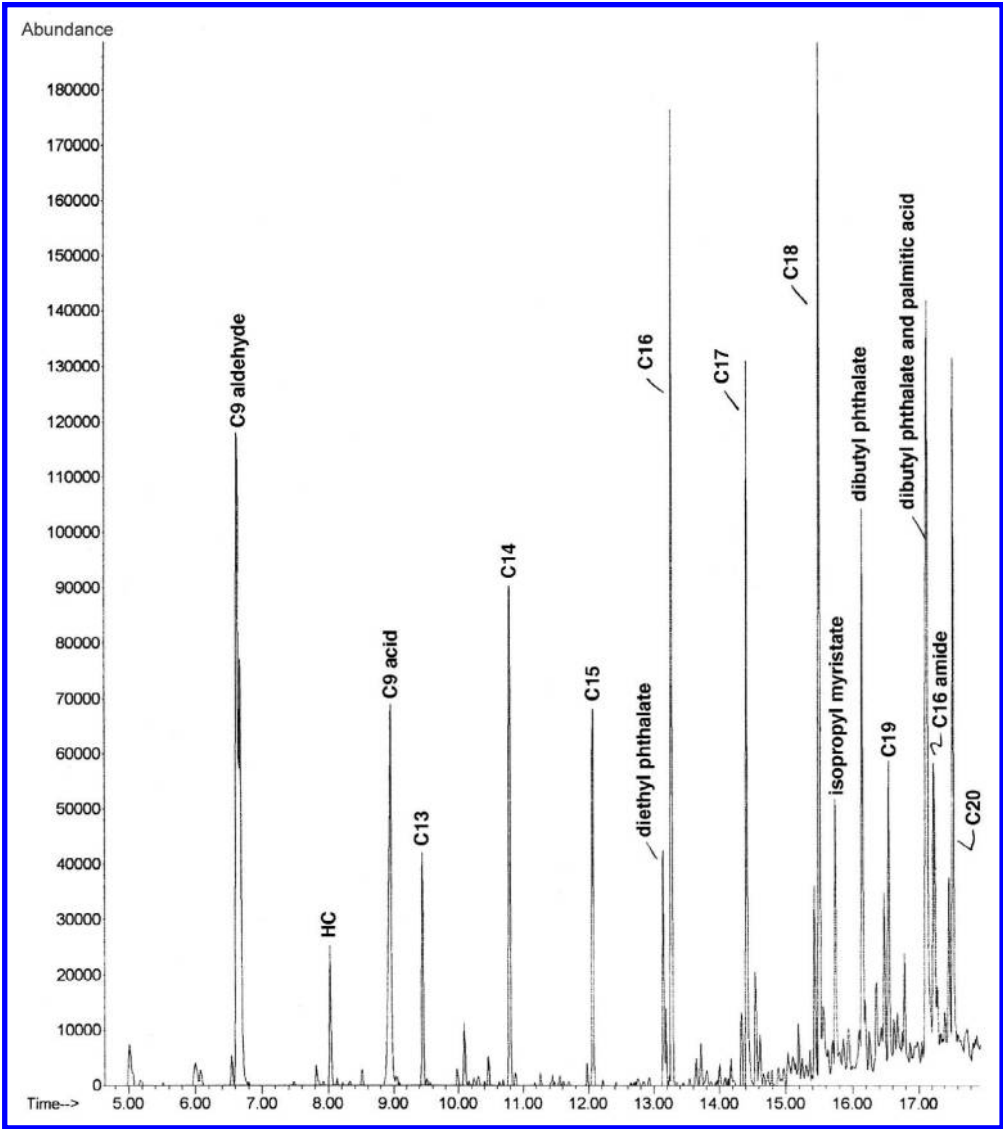


Figure 10-12 GC/MS Chromatogram of Gaylord Liner

Case Study #3: BPA-Free Coffee Cup

As part of a general survey of polymeric materials that come into human contact through packaging, toys, cooking utensils, drinking straws, and plastic utensils, a coffee cup was subjected to GC/MS analysis. This particular cup was selected because it carried a label indicating that it is “BPA-free,” as shown in Figure 10-13.



Figure 10-13 Label on “BPA-Free” Reusable Coffee Cup

The same label indicates that the cup was manufactured with 21% post-consumer plastics. The popular campaign against certain chemical compounds in food has led to production of a new wave of products, often carrying labels suggesting a certain level of purity or acceptability. In this example, the sourcing of the 21% of post-consumer plastics is not indicated. While such a label may be attractive, it seemed improbable to us that the raw materials comprising the “post-consumer recycled content” could be economically and practically analyzed and controlled. Chemical analysis by GC/MS, using thermal desorption sampling, was undertaken. The results shown in [Figure 10-14](#) confirmed the presence of BPA. The mass spectral match quality was found to be 95%, as shown in the mass spectrum presented in [Figure 10-15](#). This compares the mass spectra of the coffee cup (top) and reference mass spectrum for BPA (bottom). Several areas of the same cup were subjected to analysis and BPA was found in each case. It is not clear how this product can be claimed as being free from BPA.

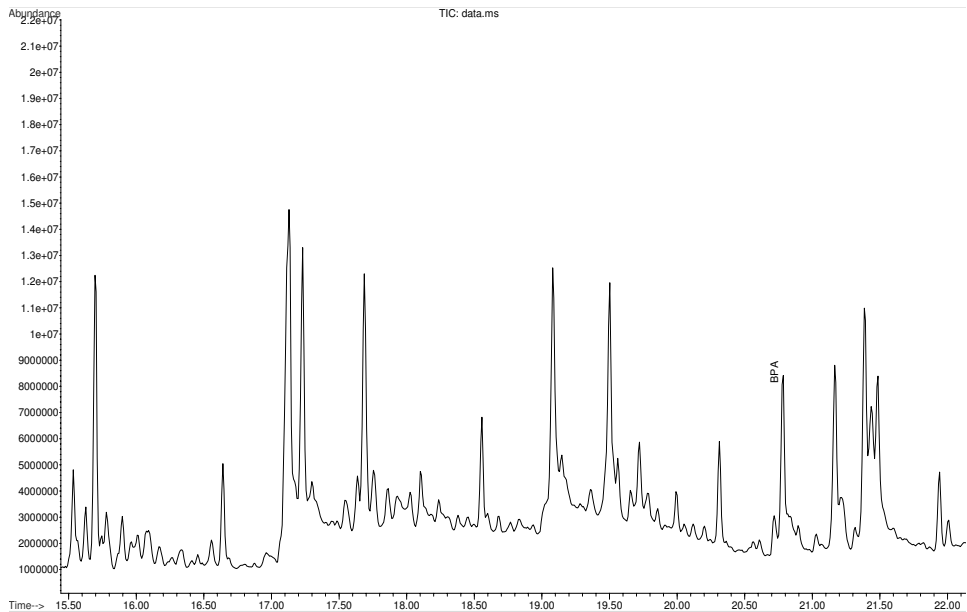


Figure 10-14 Total Ion Chromatogram of Coffee Cup Material Showing the Presence of BPA

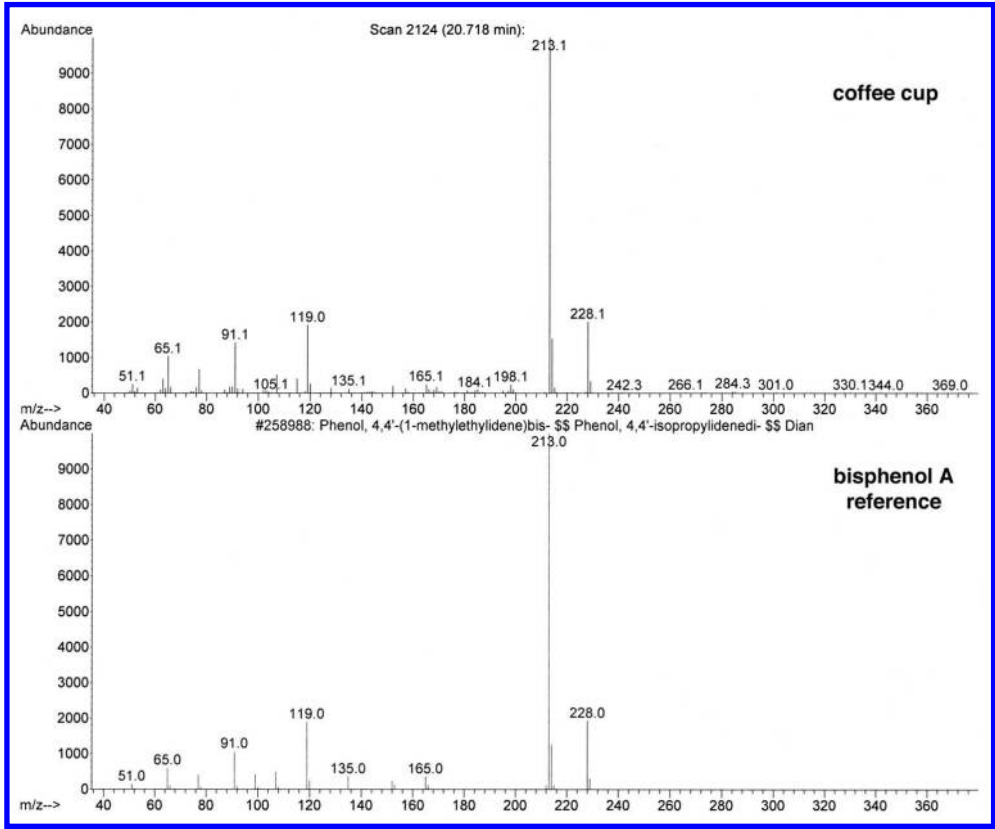


Figure 10-15 Mass Spectral Comparison of Cup Material and BPA Reference File

Case Study #4: Polymers Used in Infant Chew/Teething Toys

There are a large variety of polymeric and plastic chew/teething baby toys on the market. For obvious health and safety concerns, the polymers used for this application must be as pristine and additive-free as possible. Several manufacturers of such toys state that they produce items made from “natural” rubber and use no toxic paints or other embellishments. In addition, these “natural” products are claimed to exclude the chemicals often present in plastic toys. This is actually a false premise due to the fact that the “natural” rubber is subjected to processing and molding, which introduces adulterants such as antioxidants, lubricants, processing aides, and mold-release agents. These compounds can be incorporated into the material and may leach out during use.

The authors were asked to evaluate a well-known and popular baby chew toy which is available on-line and at a number of nationally known retail stores. Our first purchase was made online; and several portions of the toy from several different areas were subjected to thermal desorption GC/MS as described in Chapter 2 of this book.

The GC/MS results were both surprising and disturbing. Among the volatiles identified were antioxidants, processing aids, and mold-release agents. More importantly, we also identified Ziram [Zinc, bis (dimethyldithiocarbamate)], which is used as a rubber (polymer) vulcanization accelerator and a fungicide (see Figure 10-16). Ziram is published on the EPA TSCA list and is a poison by ingestion. Although Ziram is practically insoluble in water, the solubility may be enhanced by pH and enzymatic factors present in a child’s mouth. Additionally, it is an irritant to eyes and mucous membranes. The Ziram accounted for 26% of the total volatiles present in the polymer samples.

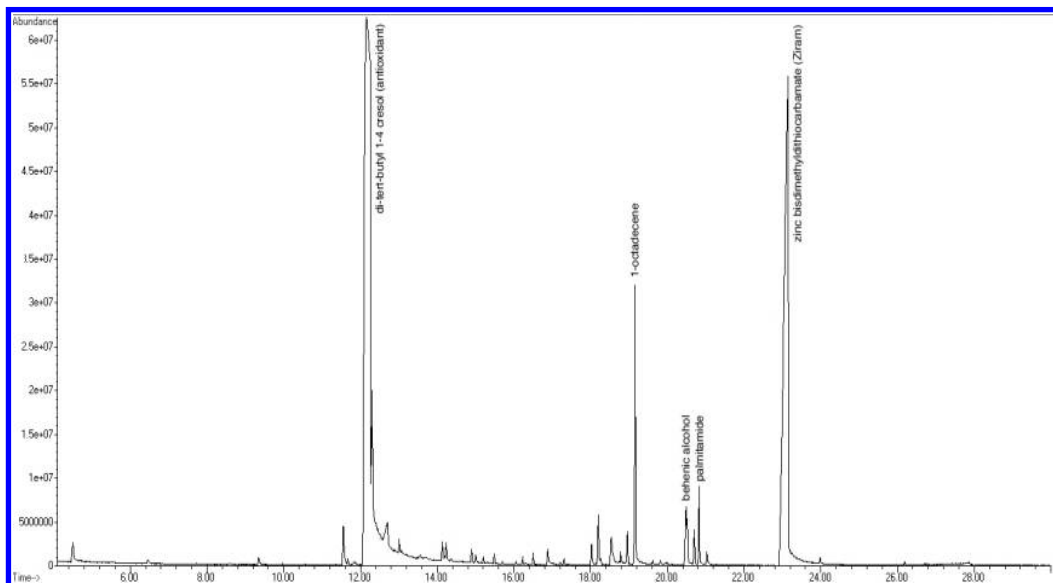


Figure 10-16 GC/MS Analysis Summary of First Chew Toy Rubber Sample

Obviously, the analysis of a single item does not equate to a trend within a product line. We were unable to locate a second item with the same lot number, so we tested a second chew toy that we purchased from a well-known baby-store chain. Figure 10-17 shows the volatiles extracted and identified in this sample. Although there was no trace of Ziram in this toy, there were a number of polymer additives including fatty acids, amines and amides that again calls into question company statements about “natural” rubber with no plastic-related adulterants.

An online survey of these types of toys revealed that counterfeit toys ('fakes', 'knock-offs') represent a well-documented problem within the industry. If our initial test results are indeed from a counterfeit toy, it represents more than just lost revenue for the manufacturer. Health and safety as well as liability issues are real possibilities. However, if the results were from a legitimately manufactured toy, then it is the responsibility of the company to ensure that the pedigree of all raw materials is accurately determined and controlled. This is essential to prevent the inclusion of unknown and potentially harmful compounds into the final product.

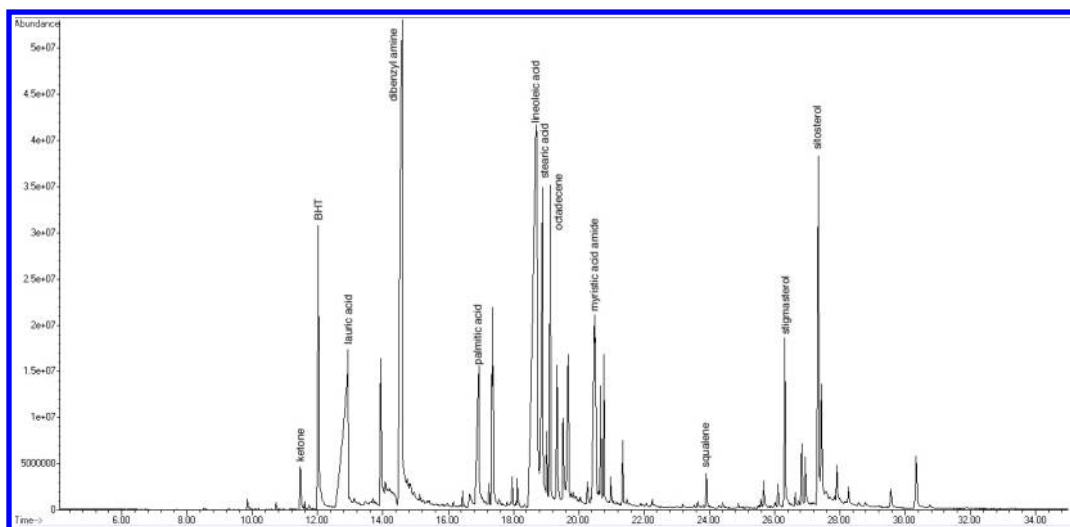


Figure 10-17 GC/MS Analysis Summary of Second Chew Toy Rubber Sample

CASE STUDIES: POLYMERS FOR ELECTRICAL EQUIPMENT APPLICATIONS

Introduction

Polymeric materials are widely used for electrical equipment applications. Use of these polymers is steadily increasing as traditional materials such as porcelain and phenol formaldehyde resins are being replaced due to weight, cost, and technical considerations. Designs of electrical equipment are based on a combination of electrical and mechanical engineering considerations. Equipment is typically qualified by standard industry and manufacturer-specific accelerated electrical stress testing in addition to mechanical testing for certain types of equipment. Polymeric materials often perform well under short-term conditions due to inherently favorable dielectric strength and low dielectric losses. However, significant experience from investigation of field-aged components shows a strong dependence on polymer formulation in achieving stable long-term performance under service conditions.

Background

Polymeric materials cover a wide range of applications for electric power distribution and transmission equipment service. These may experience relatively benign aging conditions inside of electrical equipment. In other cases, direct exposure to a harsh combination of stresses is expected. For example, an outdoor polymeric insulator will be exposed to direct sunlight conditions, extremes of temperature, exposure to rain and ice, static and dynamic mechanical stresses, electrical stresses, and the insidious effects of corona. The latter is caused by ionization of the air due to highly localized electrical stresses. This leads to production of ozone, free radicals due to decomposition of contaminants, and ion bombardment. The combined effects lead to favorable hydrolysis conditions for many polymers, accelerated by heating from high energy equipment.

Other electrical equipment is either directly buried or installed in underground conduit systems. In this type of environment, the extremes of temperature are less often experienced; however, localized and transient heating is experienced when power loads are high or when equipment runs near steam pipes, for example. In underground installations, corrosive conditions are found based on road salts, lime extraction from concrete, and other minerals that become concentrated as water dries away. Exposure to microbes, oil run-off, decaying vegetation, and other materials suggests that very stable polymers are required for this service.

The electric industry traditionally designs around and purchases equipment for a 40-year life expectation. Limited access to much of the overhead and underground equipment is unavoidable and the impracticality of temporarily removing equipment from service for inspection precludes significant opportunities for monitoring in-service performance.

Case Study #1: Electrical Insulators

Bis-phenol epoxy formulations are commonly used for outdoor high voltage insulators due to a favorable combination of good mechanical strength, excellent dielectric properties, and the ability to cast the resin around internal functional devices and electrical connections. [Figure 10-18](#) shows two examples of outdoor high voltage insulators used for capacitor switching. A review of the formulation of these insulators was conducted to predict the most favorable long-term performance among several suppliers, based on fundamental polymer chemistry principles. Analysis by GC/MS was undertaken to investigate for UV stabilizers, residual polar curing agents and curing byproducts, and other organic compounds that may adversely influence long-term aging in the field. Direct comparison based on long-term field-aging performance was not possible due to time constraints.

Chemical analysis of an insulator from one supplier indicated polymer fragments and curing byproducts, as shown in [Figure 10-19](#). In contrast, GC/MS analysis of an insulator from another supplier indicated significant differences. No traces of curing agents or corresponding breakdown products were found, thus indicating a complete curing reaction. Triphenyl phosphate flame retardant was also found in this analysis. Since devices of this type are predominantly mounted on wooden utility poles, a flame retardant formulation may provide a desirable operating margin in the event of an electrical failure. However, as shown in [Figure 10-20](#), this same insulator was also found to contain polybrominated biphenyls (PBBs), which are banned from manufacture or use in most countries. The analysis of this material protected the electric utility company from potentially inadvertent deployment of a hazardous material.



Figure 10-18 Comparison of Outdoor High Voltage Insulators

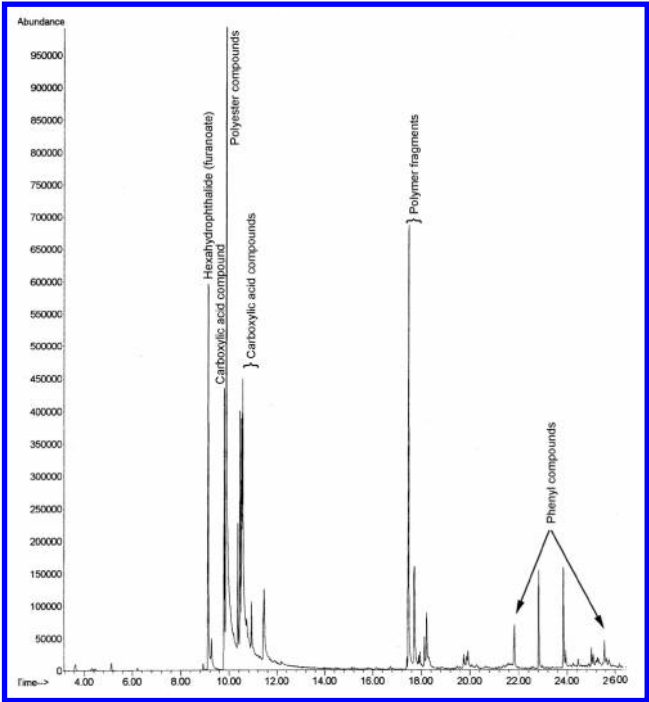


Figure 10-19 GC/MS Analysis of Insulator from Supplier A

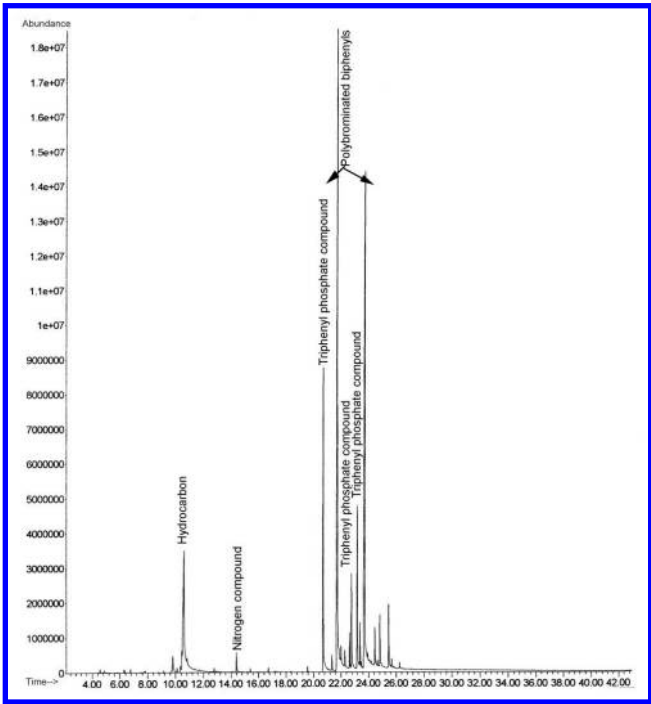


Figure 10-20 Analysis of Insulator Containing Banned PBB Material

Case Study #2: Review of Field-Aged Elastomeric Materials

Elastomer compounds are used as insulators for many electrical components. These are typically applied over fiberglass rods where load support is needed. Review of rubber formulations that have suffered significant aging damage is useful as a basis for considering alternate formulations. In Figure 10-21, a severely degraded rubber insulator is shown. This device had been in service for approximately 30 years, with direct sunlight exposure. Figure 10-22 compares another example of the same formulation where there was no direct or prolonged sunlight exposure. Based on this difference, UV degradation of the rubber compound is clearly a significant factor in reducing the useful life of this component.

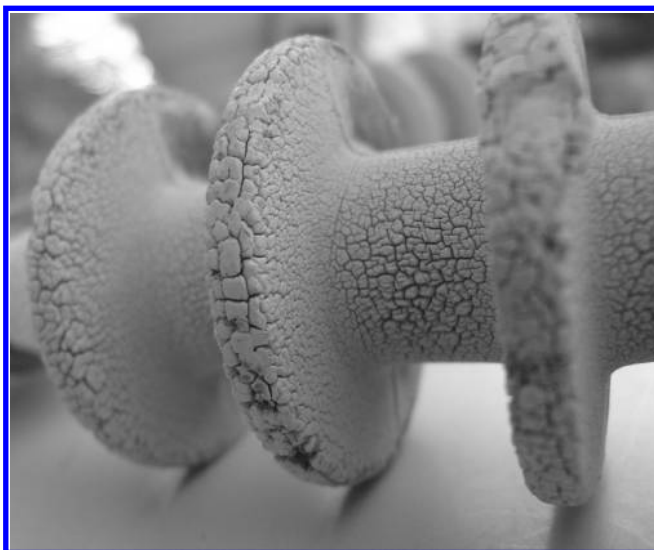


Figure 10-21 Example of Severely Degraded Elastomeric Insulator

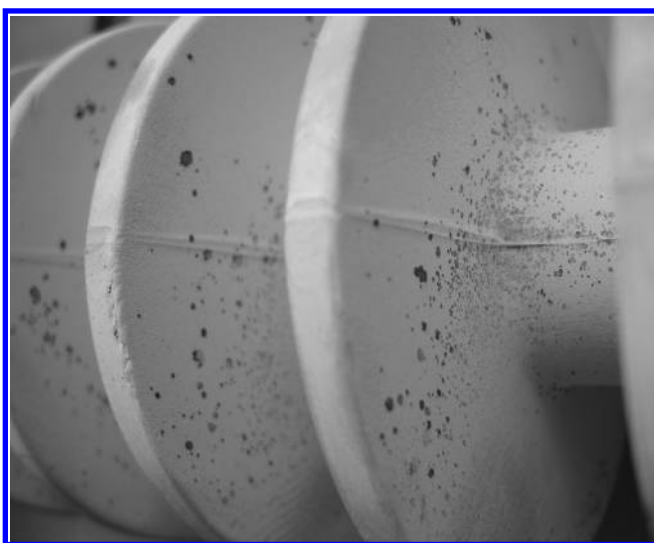


Figure 10-22 Same Insulator without Sunlight Exposure

Analysis of the degraded elastomer insulator is shown in Figure 10-23. This indicates a hydrocarbon rubber, based on the homologous series of hydrocarbon peaks, plus myristic, palmitic, and stearic acids. This sample was obtained from the core of the device, where significant weathering had not damaged the material. Hydrocarbon rubber is very susceptible to UV-induced chain scission and protection is required to extend useful service life. In this example, the grey color is imparted by silicate clay. This adds strength to the rubber. However, it is inefficient as a UV absorber. Further, GC/MS analysis indicates that no coupling agent (vinyl silane, for example) was used to promote chemical bonding between the rubber and clay. Fatty acids were added as a processing aid for mixing of the rubber compound. These are easily hydrolyzed by water in combination with UV radiation. As the fatty acids are removed, the free volume of the elastomer increases, thus increasing the specific surface area available for UV interaction. The absence of a clay/coupling agent system also leads to increased free volume as the elastomer degrades.

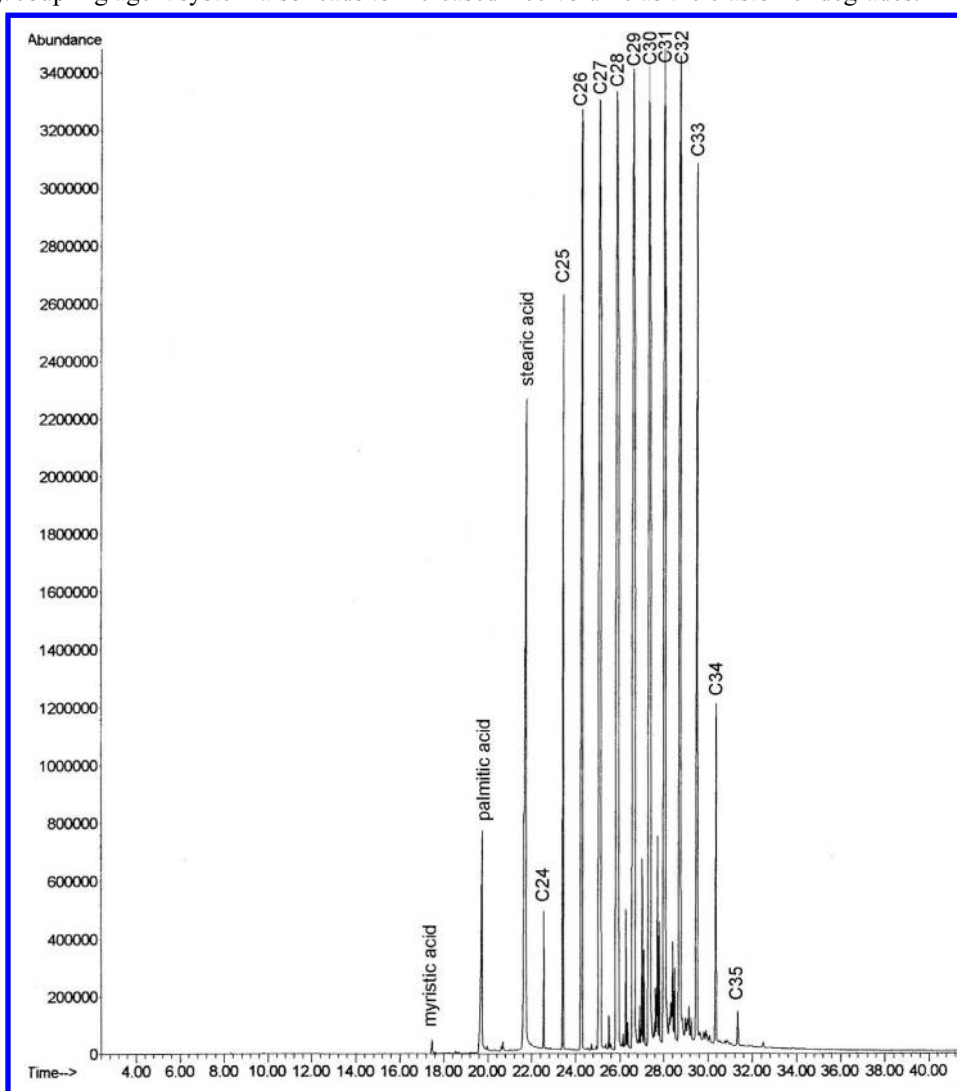


Figure 10-23 GC/MS Analysis of Poor Performing Rubber Compound

Figure 10-24 presents the GC/MS analysis of a rubber formulation for an elastomeric insulator for devices to replace those that had been characterized after field-aging. In this example, a high

quality silicone rubber was selected for inherent resistance to oxidation and UV damage, plus favorable dielectric properties. GC/MS analysis of this elastomer confirmed pure silicone rubber as the base polymer plus Tinuvin P, a UV absorbing polymer stabilizer. To reduce cost, many suppliers provide “silicone rubber” components that are often combined with butyl or nitrile rubber to reduce cost.

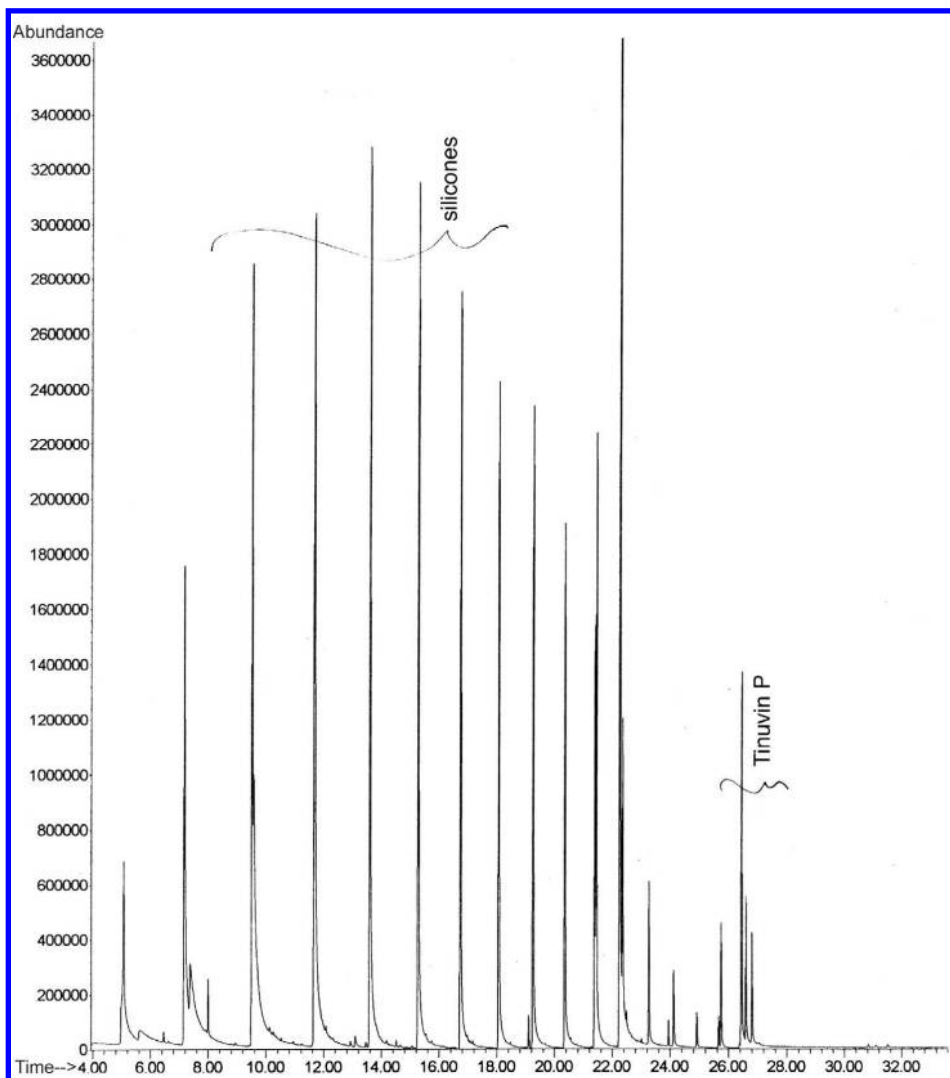


Figure 10-24 Composition of Preferred Silicone Rubber Formulation with UV Stabilizer

Case Study #3: Performance of Polymeric Seals

For electrical equipment, polymeric seals are used for many electrical applications including oil retention, nitrogen or sulfur hexafluoride gas pressure barrier, moisture exclusion, and lubricant retention. Mechanical seals and O-rings are typically specified based on polymer type (i.e., silicone, buna, Viton) and durometer hardness value. The latter is a measure of the elastic resilience of a seal. The base polymer is chosen on the basis of compatibility with the selected contact material. Catalogs from seal suppliers are devoid of any significant technical details regarding formulation. For example, if a large cover that is sealed with an O-ring must be opened

periodically for inspection, adhesion of the O-ring to the mating surfaces cannot be tolerated. Figure 10-25 presents the GC/MS analysis of an O-ring from such an example, where a cover of 1.5 m diameter, weighing more than 200 kg must be opened for periodic inspection of internal components of an electrical circuit breaker.

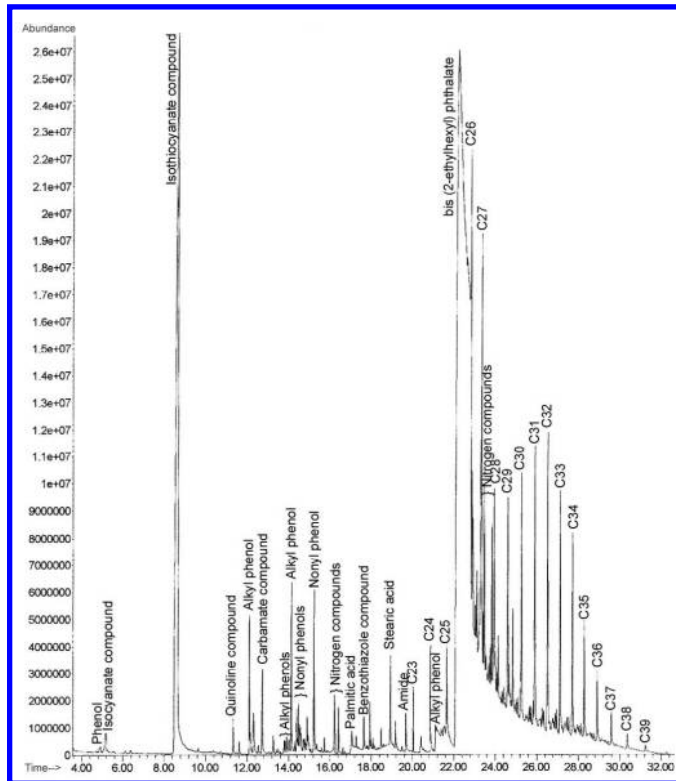


Figure 10-25 Sticky O-Ring Analysis by GC/MS

The rubber formulation is complex and includes residual thiocyanate curing compounds, alkyl phenol antioxidants, bis (2-ethylehexyl) phthalate plasticizer, and hydrocarbon fragments from the butyl rubber base polymer. Phthalate plasticizers are added to improve the flexibility and reduce hardness in rubber compounds. However, these have limited solubility in most polymers. A plasticizer of this type migrates to the free surface where it becomes trapped against the metal sealing surface. Hyper-plasticization of the O-ring surface results, leading to a very tacky surface that adheres well to metals. The O-ring chosen is not suitable for this application. A material requiring less plasticizer would be a better choice to correct this issue.

CASE STUDIES: QUESTIONED ANALYTICAL PROCEDURES

Introduction

As with all analytical procedures, the analyst must make judgments regarding a number of factors such as sample preparation, extraction solvent, extraction temperature/time, and methods of sample handling and concentration. All of these decisions require some knowledge of the materials under analysis; otherwise, the results may not be indicative of the original materials and their components. Further, the application of the analysis results must be carefully considered in context of the application. When testing polymeric compounds for toxic release under fire conditions, it is reasonable to pyrolyze the sample during analysis. It is not reasonable, however, to thermally decompose a prospective material that will be used for an application such as a toy or toothbrush. GC/MS is a powerful analytical tool and, as with any analytical technique, proper application is paramount.

Case Study 1: Benzene in Blister Packaging Materials

Many tablet medications intended for unit dose applications are protected by the familiar blister packs, an example of which is shown in Figure 10-26. These are typically manufactured with laminated materials that consist of a transparent polymer, an aluminum foil, and an interfacial adhesive. There are many variations of this construction. The transparent polymer layer is first “dimpled” with a heated die to produce the tablet cavities. The web material, consisting of the aluminum foil and adhesive, is thermally bonded under pressure to the perimeter of the cavities and the tablet is inserted. This is a continuous process in which the line speed, compression force, and temperature must be controlled to assure a hermetically sealed package.



Figure 10-26 Example of “Blister Pack” Pharmaceutical Packaging for Consumer Applications

During development of a new packaging system to hold dry powder medications within a blister package, problems were encountered with drug adhering to the blister walls after drug release. This problem was researched by GC/MS. The antioxidant was found to be “blooming” to the surface of the transparent blister pack layer and acting as an electrostatic “adhesive.” This type of

antioxidant was eliminated from the raw material and substituted with a grafted antioxidant. During the course of the analyses, however, one laboratory reported that it had identified benzene in the shell layer. This was not confirmed by our analyses nor those conducted by the pharmaceutical company and the packaging materials suppliers. The occurrence of benzene in the packaging of an inhalation medication is of great concern, so the dry powder delivery system development program was halted until the benzene source could be determined and eliminated, if real. The organization that found benzene insisted that its results were correct and further opined that benzene was originating from motor vehicle exhaust in a loading dock area where the packaging materials had been briefly stored. The absence of any other vehicle exhaust products went without explanation. Since the product composition is critical to patient safety, the basis for benzene detection required investigation.

Direct gas sampling from the contents of the blisters was conducted with a gas-tight syringe. Blister pack headspace gas was sampled across the full range of blister pack processing conditions, with respect to line speed, compression force, and temperature. The chromatogram presented in Figure 10-27 and the mass spectra shown in Figure 10-28 show that no trace of ion 78 (benzene) was found. The only compounds detected were those associated with the adhesive layer on the metal foil.

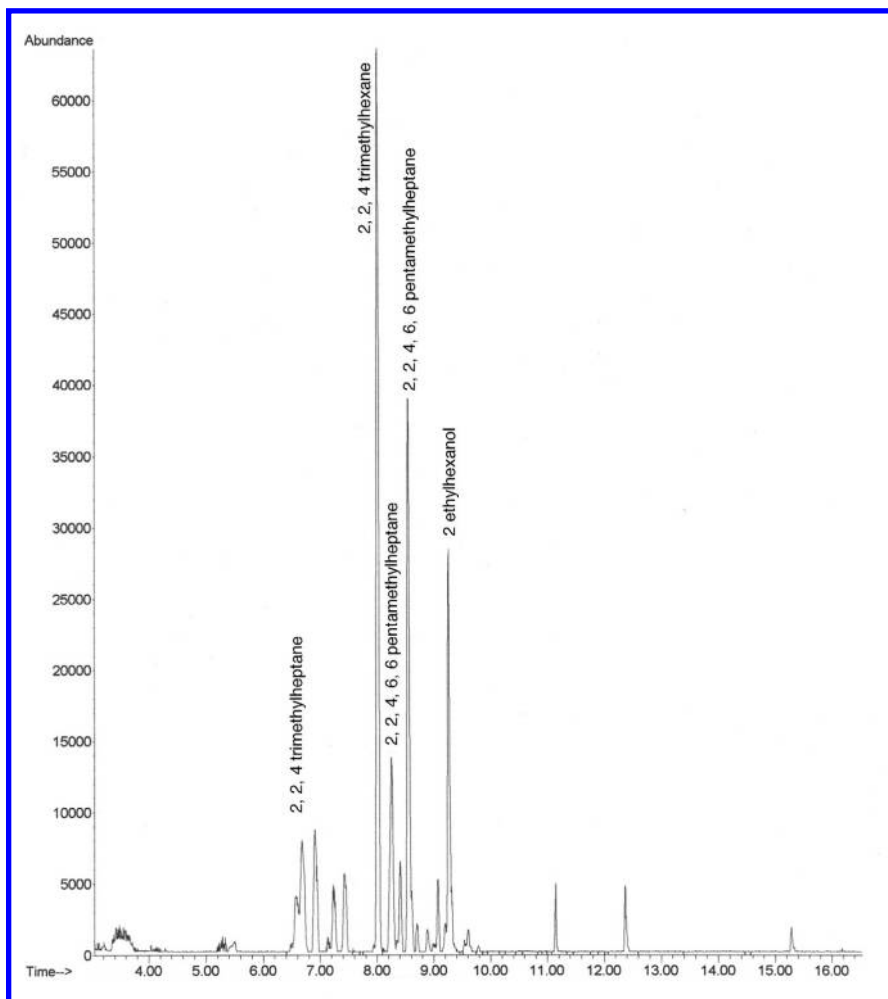


Figure 10-27 GC/MS Analysis of Headspace Gas from Blister Pack Cavity

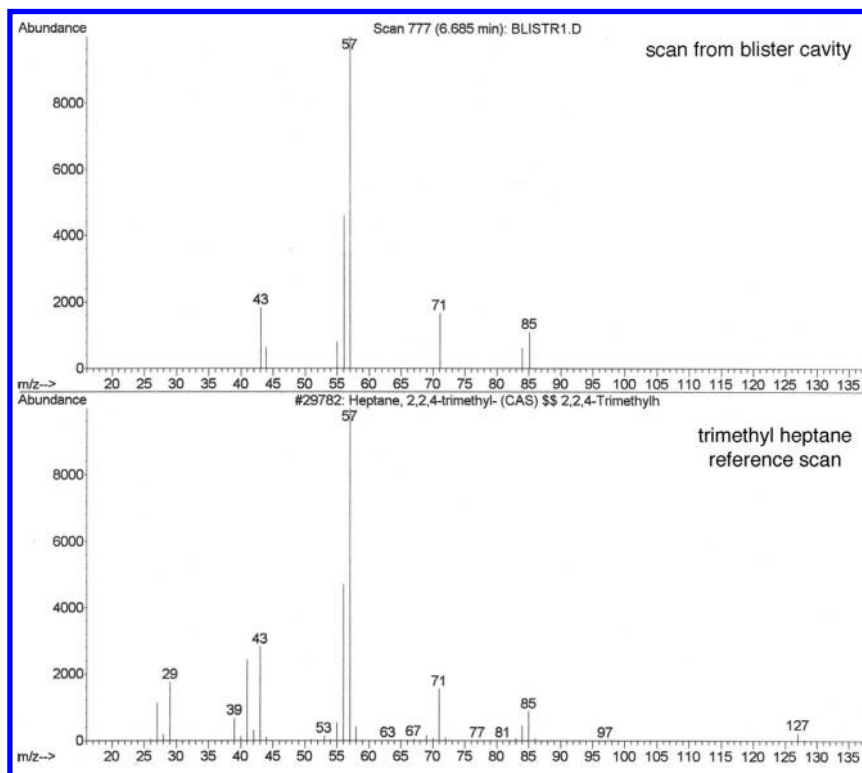


Figure 10-28 Mass Spectral Data showing Absence of Ion 78

Following a review of the discrepant laboratory's methodology, it was clear that the samples had been analyzed with a thermal desorption cell that was designed in-house. A review of the design illustration, heater placement, and thermocouple location suggested that the temperature of the interior surface of this desorption cell may be considerably above the indicated temperature. To investigate this possibility, samples of the web material were thermally desorbed at various temperatures, ranging from the agreed temperature of 180°C to 300°C in 20°C increments. At 250°C, benzene was detected, based on a single ion mass (SIM) scan for ion 78. This would be expected from thermal decomposition of the polymer. Since the web materials were never heated above 130°C during processing, the anomalous benzene finding was determined to be an artifact created during the analysis procedure.

Case Study 2: Toxic Material in Medication Container Lining

Sensitive pharmaceutical preparations are typically protected against direct contact with metallic delivery containers by application of a spray-in-place inert polymeric liner. These coating materials typically have low surface energy and a smooth surface to prevent separation of the active ingredient from the carrier. Application processes typically include a post-spray heating cycle to dry the coating or to initiate a crosslinking reaction. Long-term retention of adhesion to the container walls and long-term chemical inertness are absolutely required for any such coating materials.

In one study, a novel coating system was developed to improve on commercially available systems that included solvents, curing agents, plasticizers, and monomers. The replacement coating system was developed with highly refined monomers derived from food packaging coatings, and then

crosslinked with benzoyl peroxide. The coating material was developed and the application process was tuned to remove all traces of residual ingredients. Extraction studies with medications and their solvents indicated no trace of extraction products from the coatings. During independent testing of the containers, commercially available testing indicated the presence of benzil extracted from the coating material. This result was contrary to the development work that was carried out with the coating manufacturer and customer. Further, analysis results indicated the presence of organic compounds that were not associated with the coating materials or even with their precursor ingredients. Typical analysis results that we and the manufacturer obtained for this coating material are presented in Figure 10-29, showing data for canisters filled with ethanol and aged at 60°C for 30 days. An example of one of the commercial analyses for this same coating is shown in [Figure 10-30](#). An investigation was undertaken to provide a basis for explaining the discrepant analysis results.

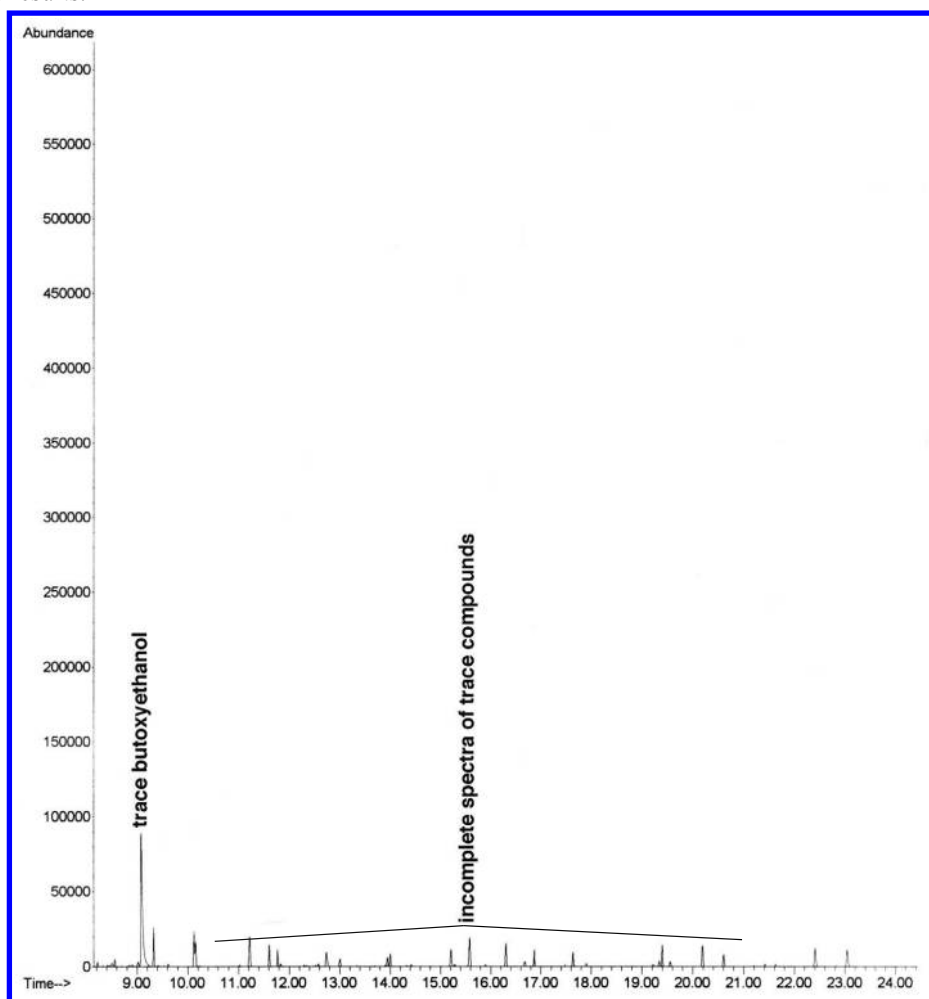


Figure 10-29 GC/MS Analysis of Ethanol-Extracted Canister Coating Material

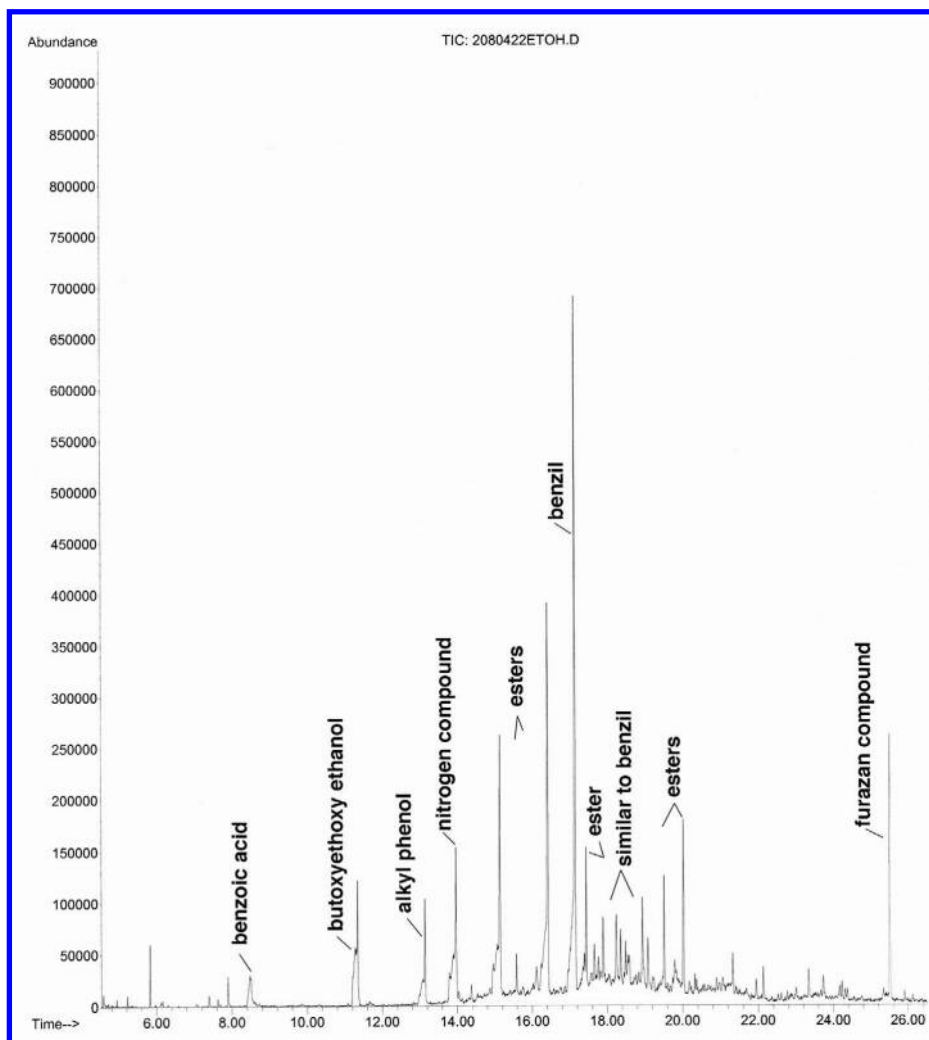


Figure 10-30 Commercial Analysis Summary of Canister Coating Material

The analyses that were conducted during the coating and process development efforts included 6-month and 1-year tests in which active pharmaceutical formulations and placebo formulations were packaged into trial containers and aged at 60°C, with periodic shaking. Additional containers were filled with polar and non-polar solvents and aged for the same period. These solvents included ethanol and the hydrofluoroalkane propellant/solvent. Analyses of the contents were conducted at regular intervals using GC/MS to check for any organic compounds that would indicate coating decomposition. The acrylic coating material in this example was crosslinked with benzoyl peroxide. The coated cans were processed at 220°C and thermally desorbed at this temperature for 26 minutes immediately following coating.

A review of the commercial laboratory analysis procedure was initiated. Sampling from the coating inside the cans began with solvent filling and ultrasonic agitation for 2 hours. The solvent was then removed and concentrated 100:1 by evaporation in an oven, using a non-covered glass container. The concentrated extract was then directly injected into the GC/MS injection port at a temperature of 330°C. We became immediately concerned when reviewing this protocol since the

coating material thermally decomposes at 260°C, as shown in our analyses. Ultrasonic agitation was reviewed. A copper sulfate solution was used to determine the coating integrity post-agitation. As shown in Figure 10-31, the coating had been physically removed by the intense ultrasonic energy that was concentrated geometrically at the base corner of the containers. The copper sulfate darkens the exposed areas of the aluminum canister. The extract was found to contain particles of the coating material. This was not filtered immediately prior to injection, as we do regularly to exclude non-dissolved materials, using a filtered syringe as shown in Figure 10-32.

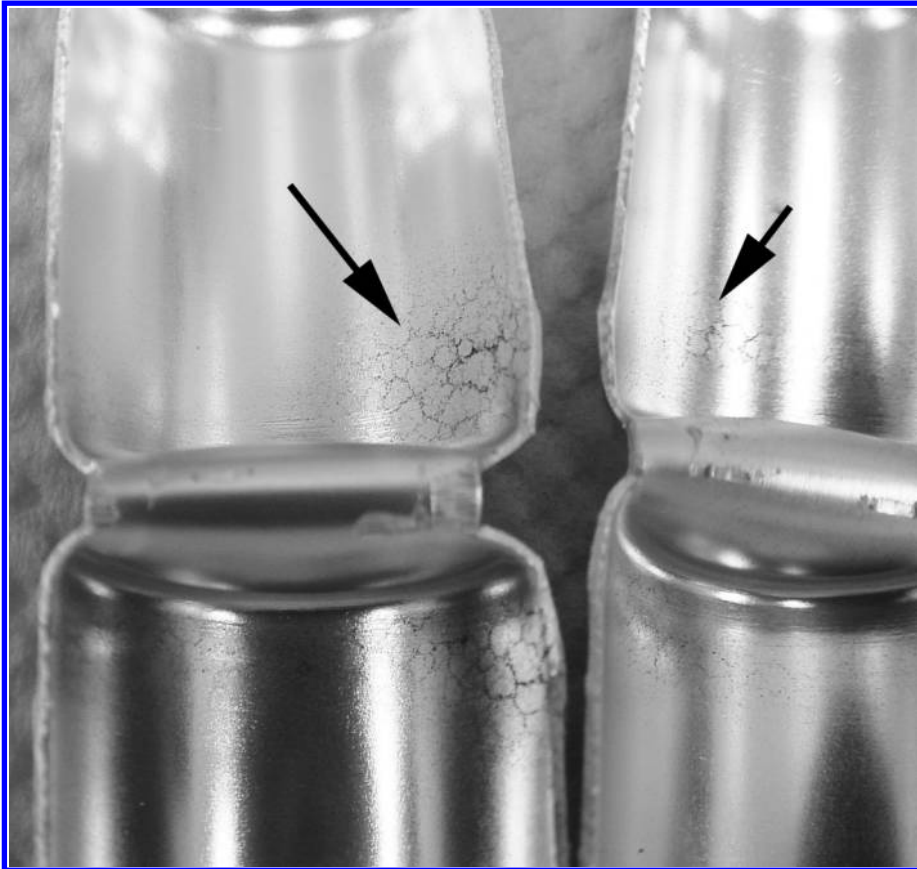


Figure 10-31 Canister Inner Surface Stained to show Coating Disruption



Figure 10-32 Consolidated Injection Syringe and Filter

By replication of the analysis procedures followed at the outside laboratory, we were able to replicate most of the unexpected results. The nitrogen peak, for example, was found to originate from thermal decomposition of the injection port septum at excessively high temperature. The esters originated from thermal decomposition of the sample base polymer. Butoxyethanol and furazan were found in the ethanol following concentration at a ratio of 100:1. In summary, the analysis was conducted by direct injection of particles of coating material, at a temperature above the onset of thermal decomposition for this polymer. The injection port temperature was sufficiently high that the septum began to decompose, contributing additional confusion into the analysis.

This case study has been included to illustrate an example of how an “independent” analysis may become a problem if there is no prior dialog and agreement on the extraction and analysis approach. Many times, commercial laboratories feel obliged to “stress” food and drug contact materials to reveal possible weakness or limited margins. It is imperative that any analysis not be conducted using conditions that cause the material under investigation to decompose and become non-representative.

APPENDIX A

Chromatograms

This appendix includes the Total Ion Chromatograms (TICs) from which the mass spectral data was obtained.

For some compounds, such as the aroclors, the pattern recognition of the chromatogram can be much more informative than the mass spectral information.

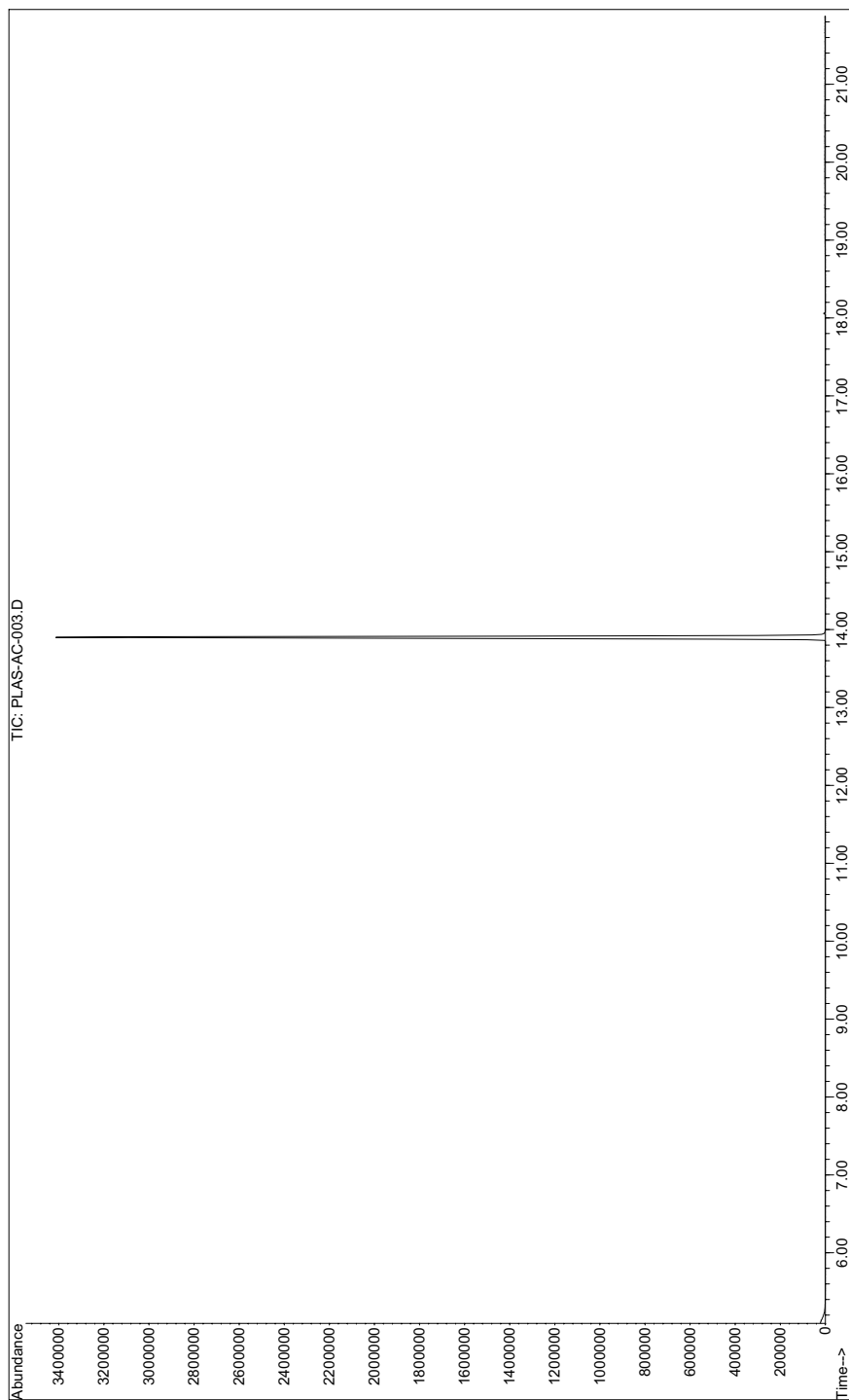
As much as possible, each chromatogram was obtained under the same instrument conditions to allow comparison between the different compounds.

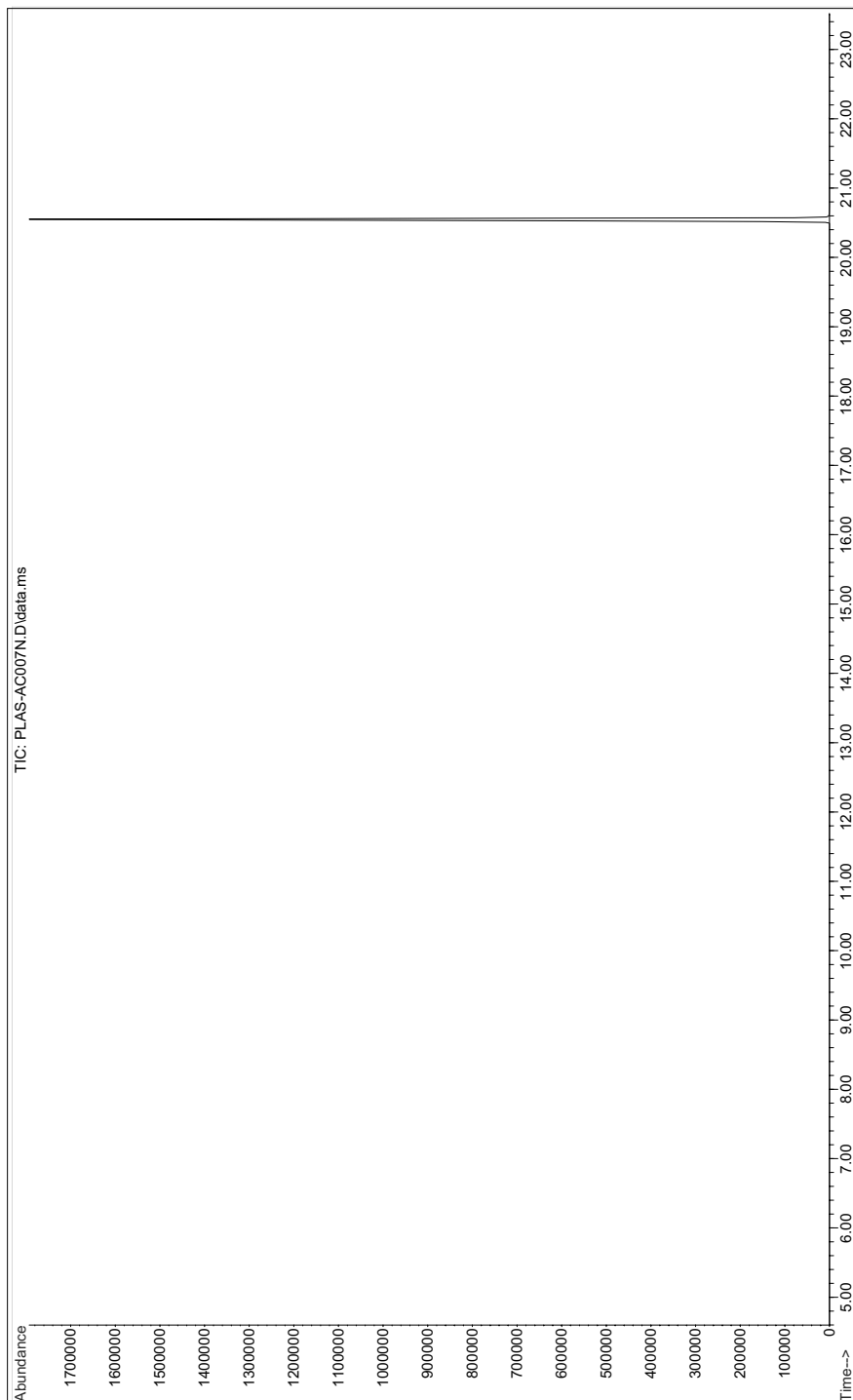
Analytical Information

Chromatogram for Accelerator BBTS - PLAS-AC-003

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

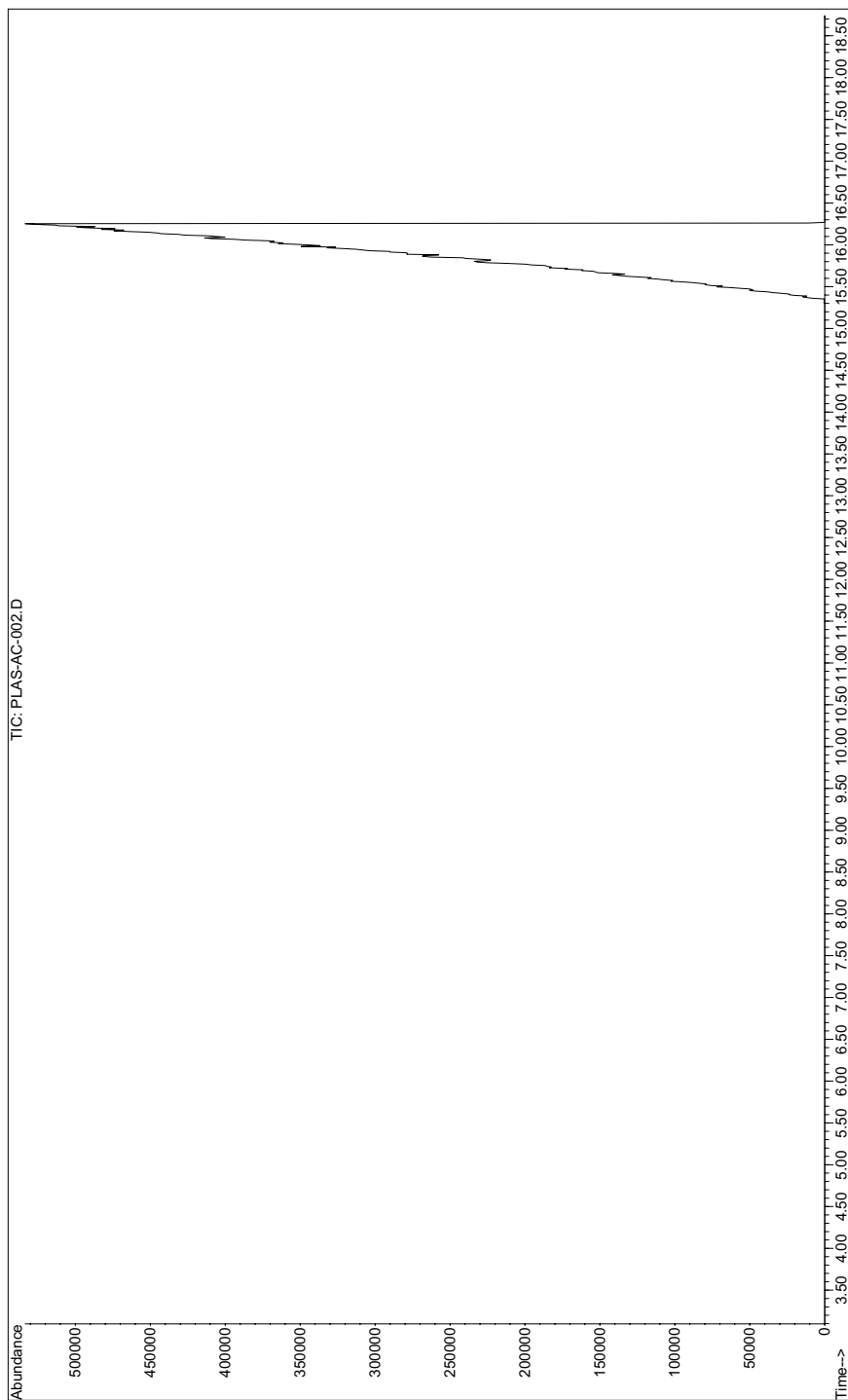
Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for Accelerator CBTS - PLAS-AC-007****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for Accelerator ETU-22 PM - PLAS-AC-002****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

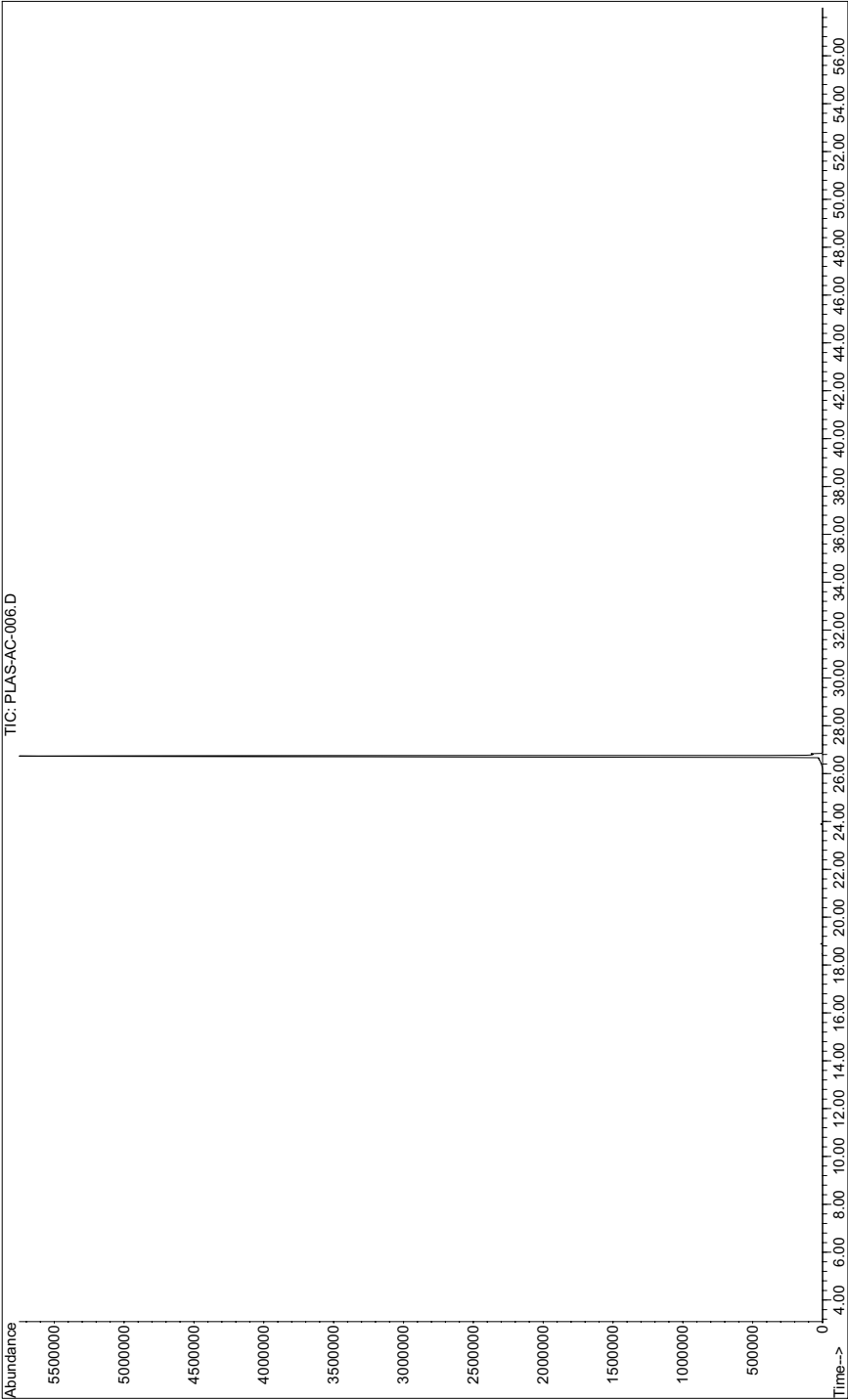
Inj Temp=250 °C, Det=MSD

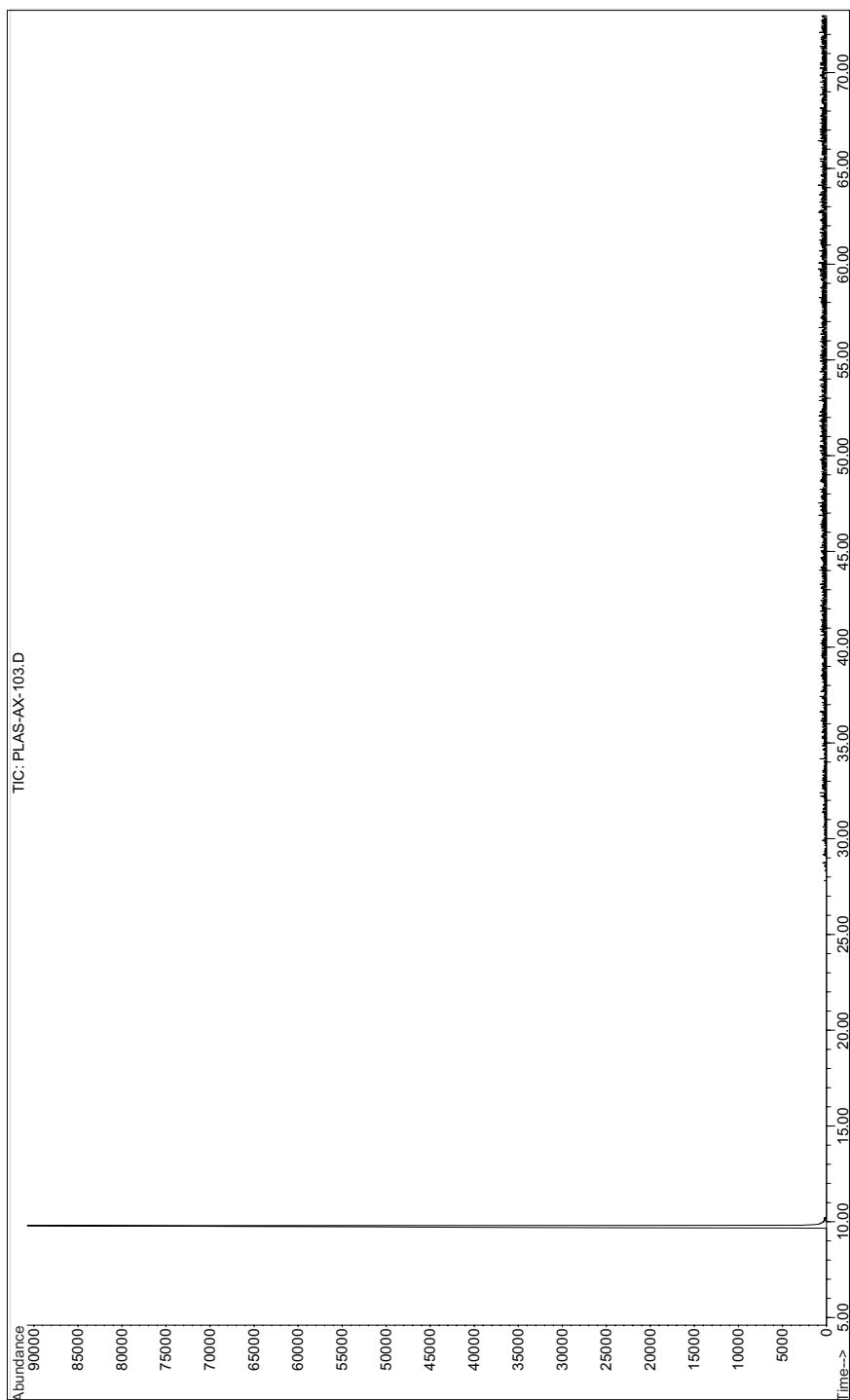


Analytical Information

Chromatogram for Accelerator EZ and EZ-SP - PLAS-AC-006

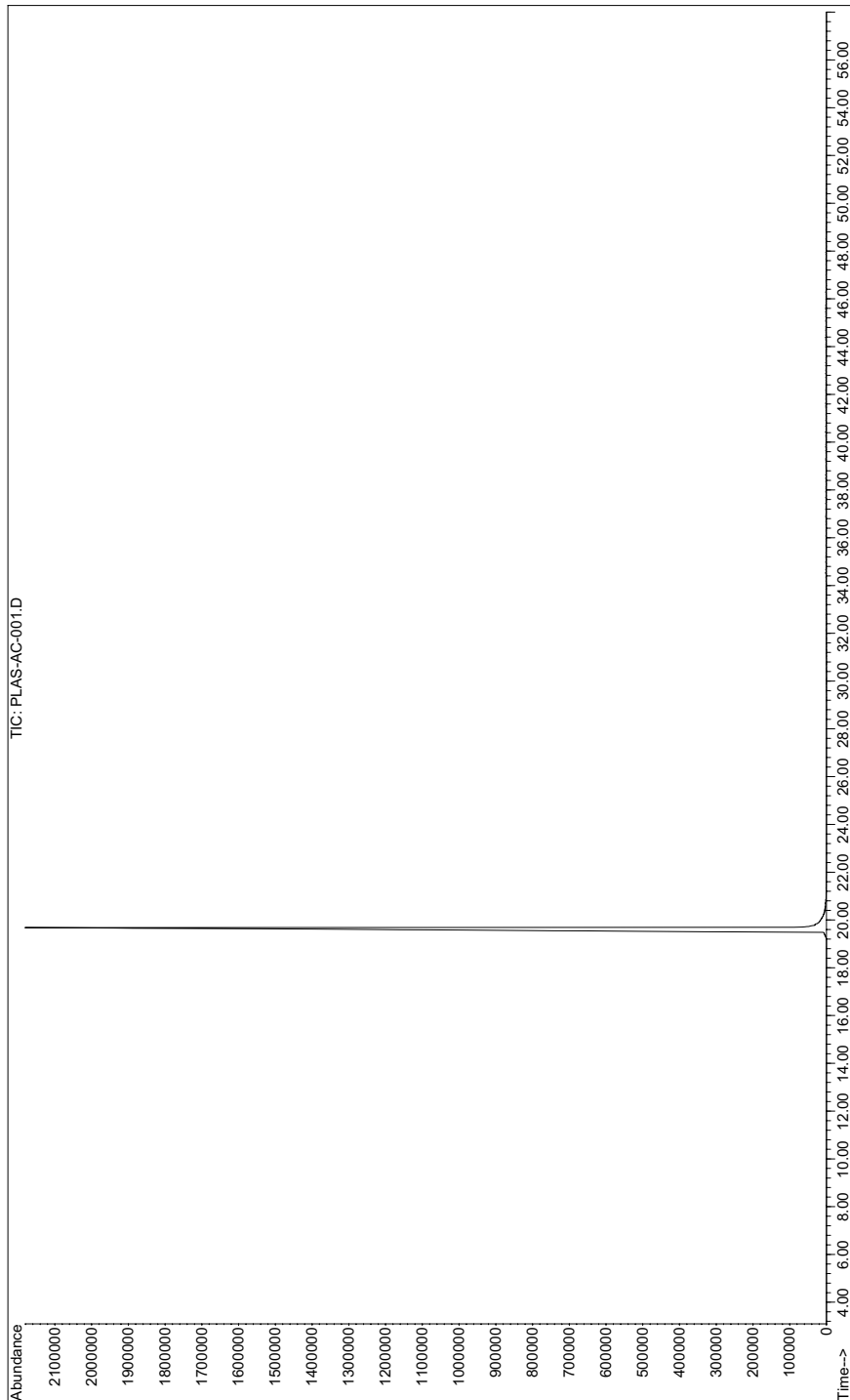
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *N,N'*-Diethylthiourea - PLAS-AX-103****Analytical Conditions Summary** 0 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for Accelerator MBT, MBT/MG - PLAS-AC-001****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD

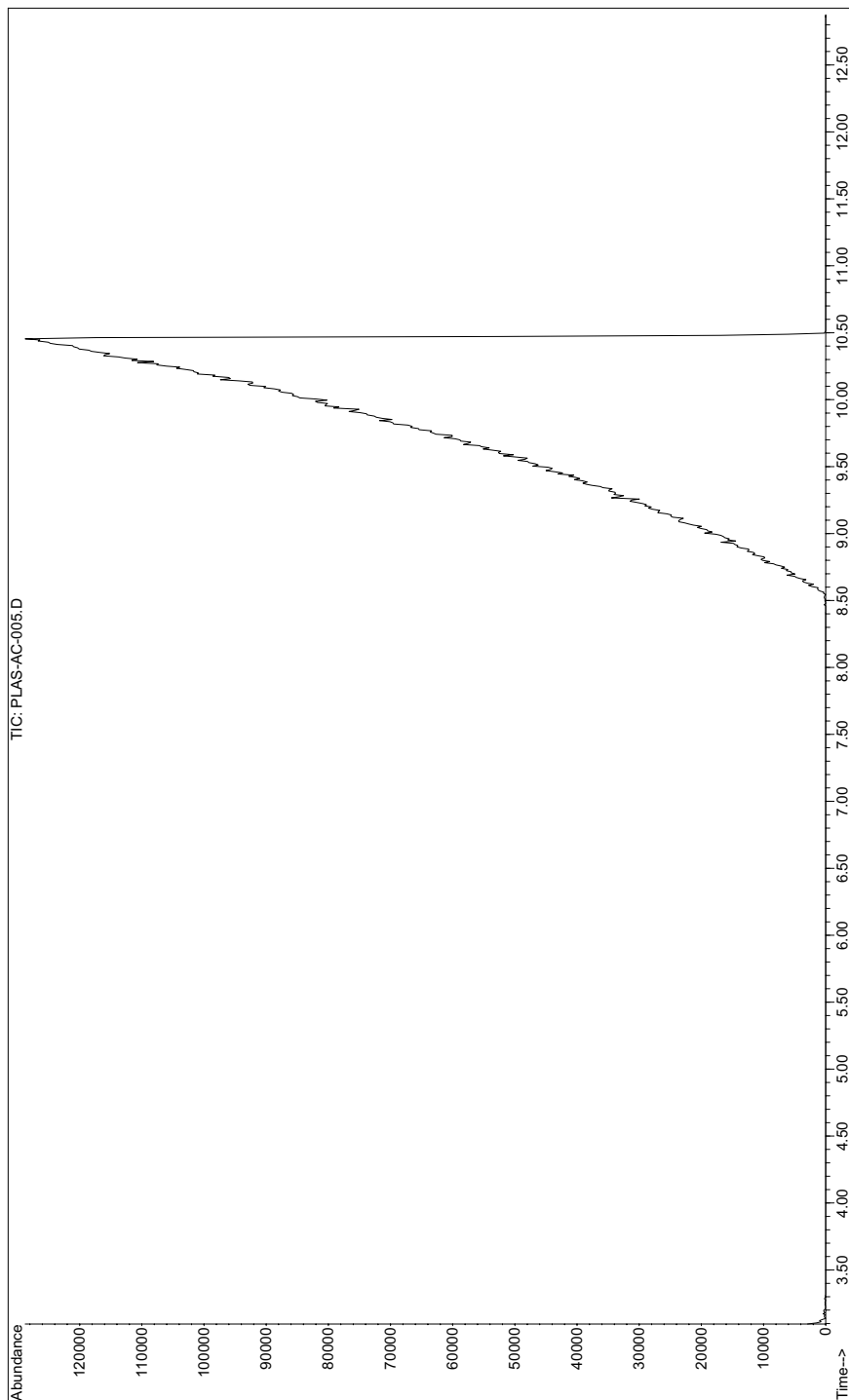


Analytical Information

Chromatogram for Activator OT Urea - PLAS-AC-005

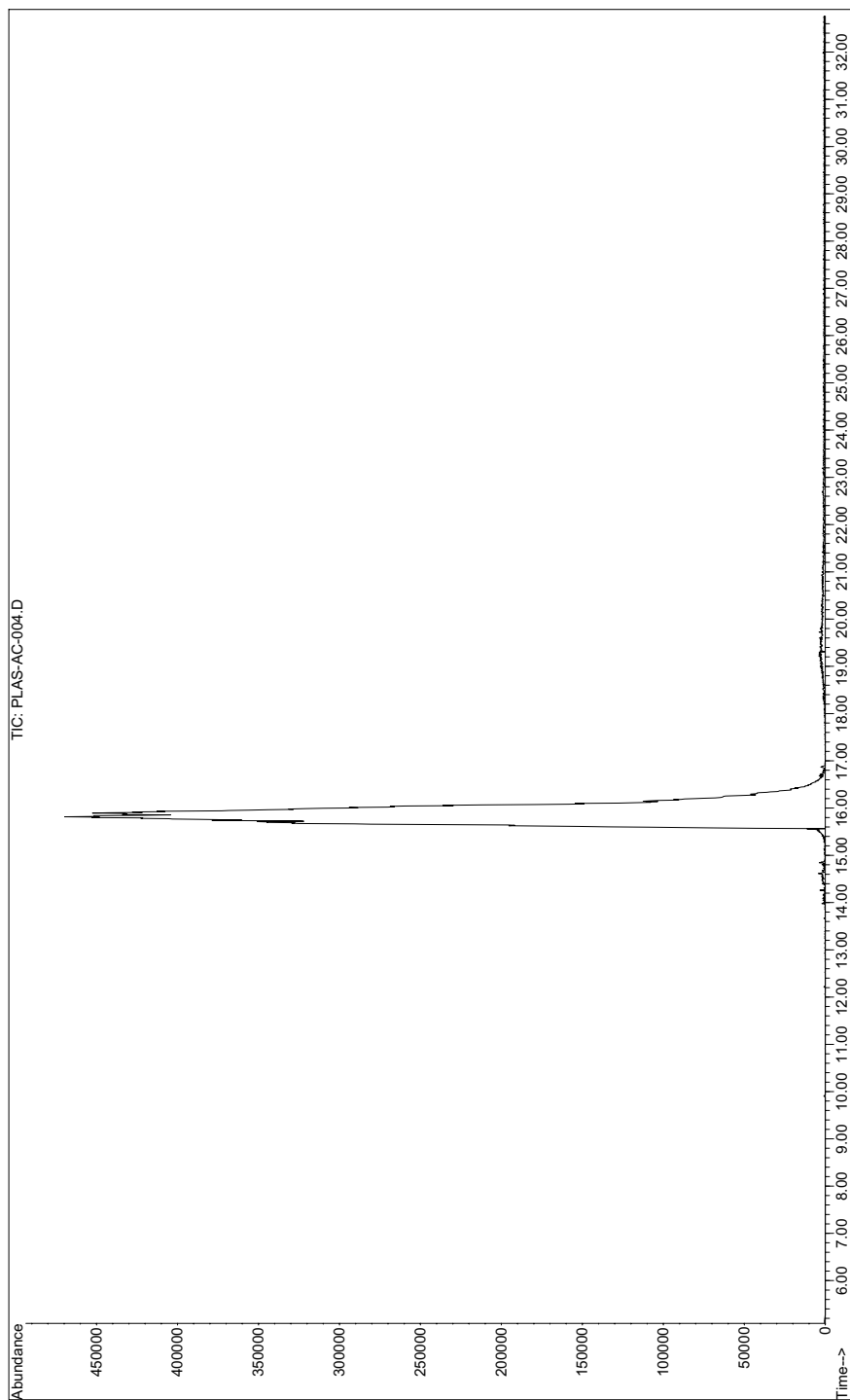
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD



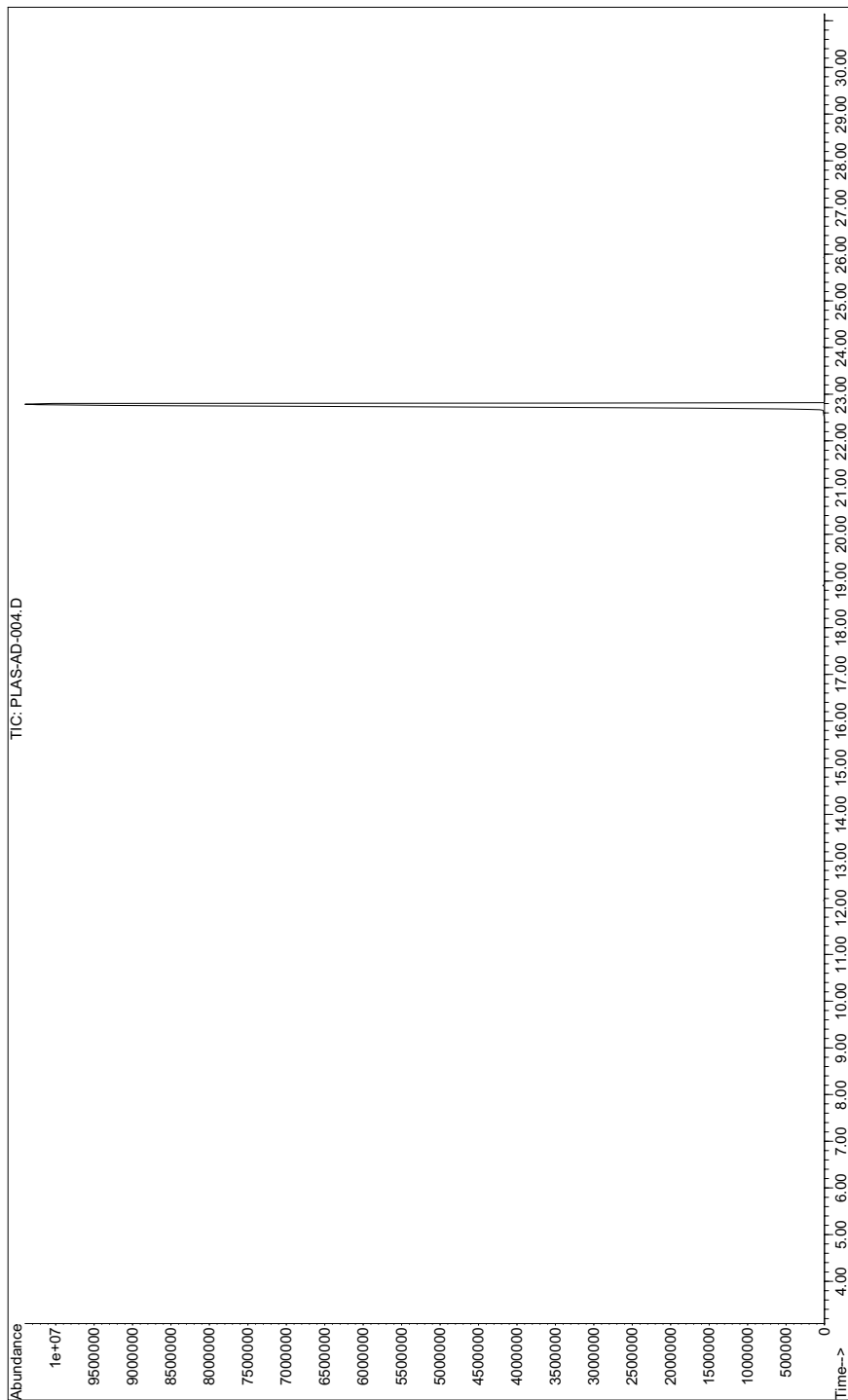
*Analytical Information***Chromatogram for *Cure-Rite®* IBT - PLAS-AC-004****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

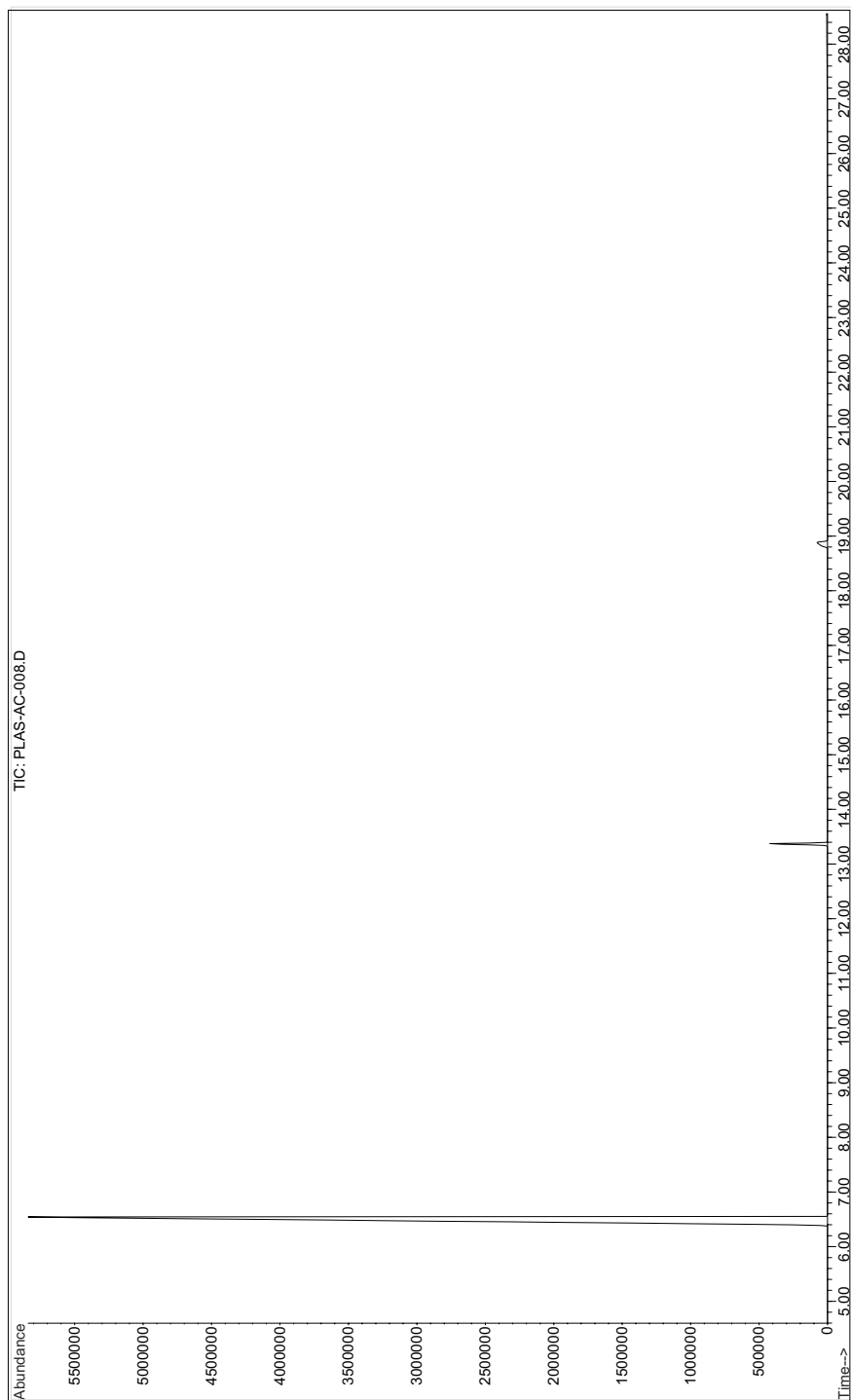
Inj Temp=250 °C, Det=MSD

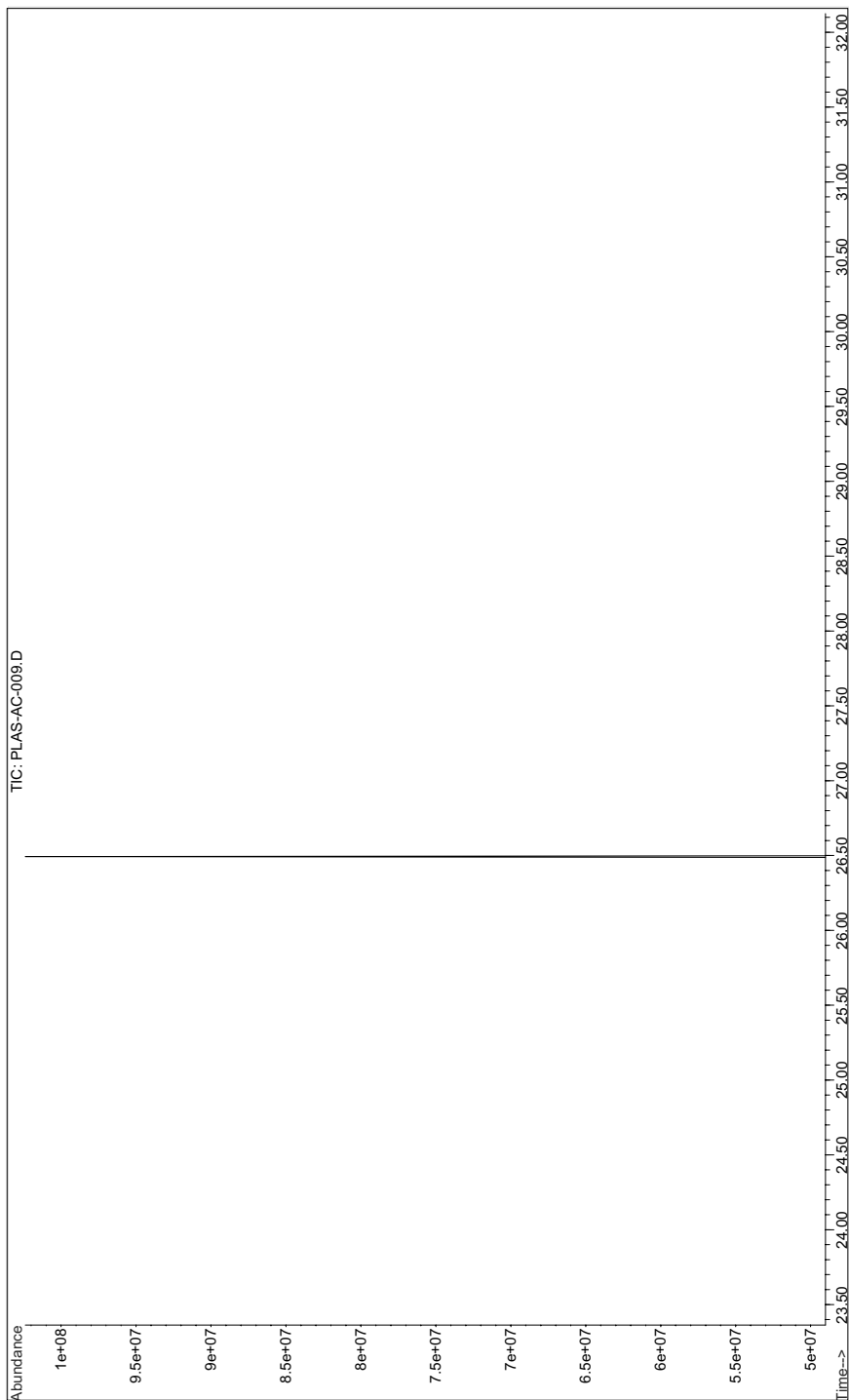


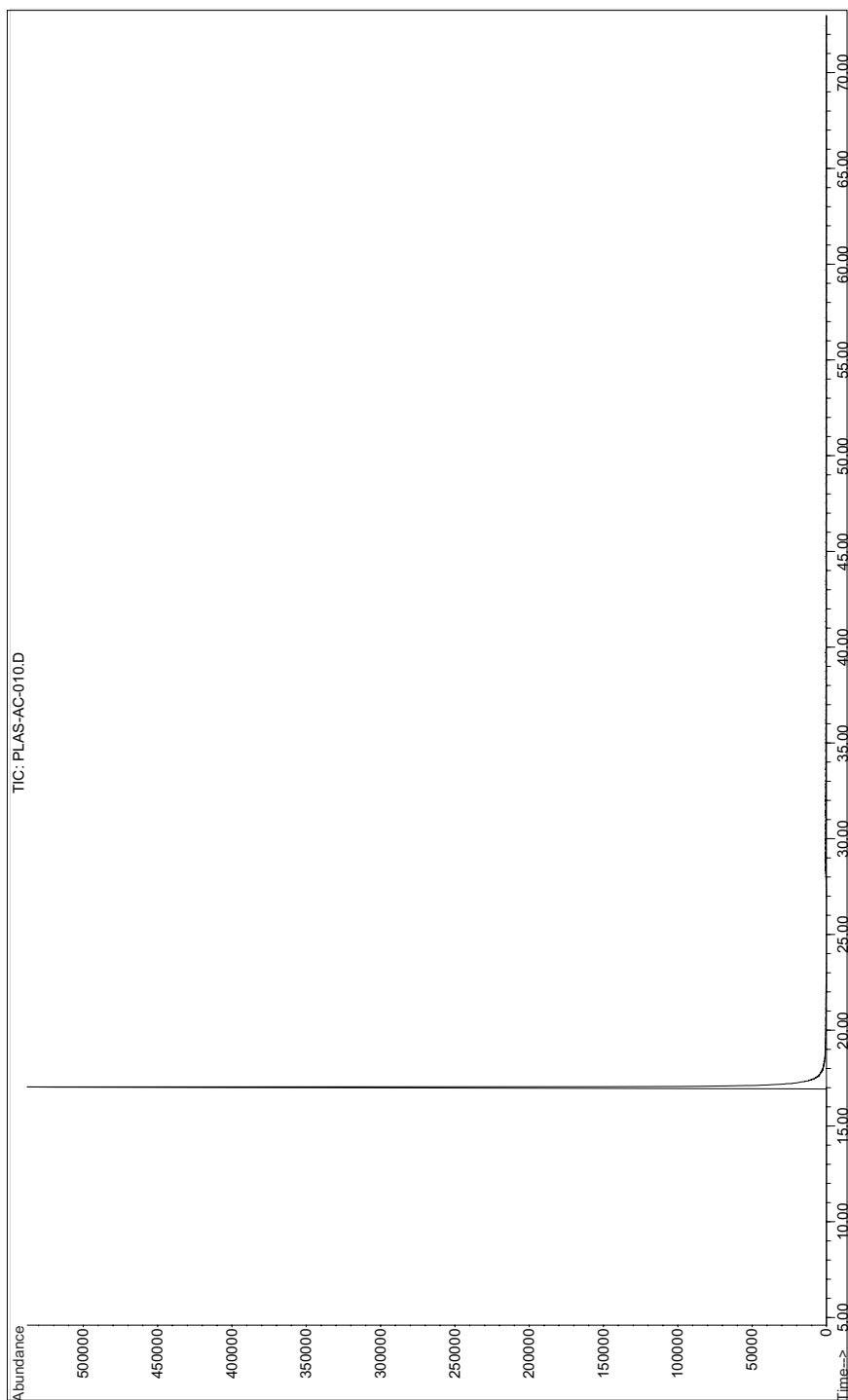
*Analytical Information***Chromatogram for *Santoflex*[®] 6PPD - PLAS-AD-004****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

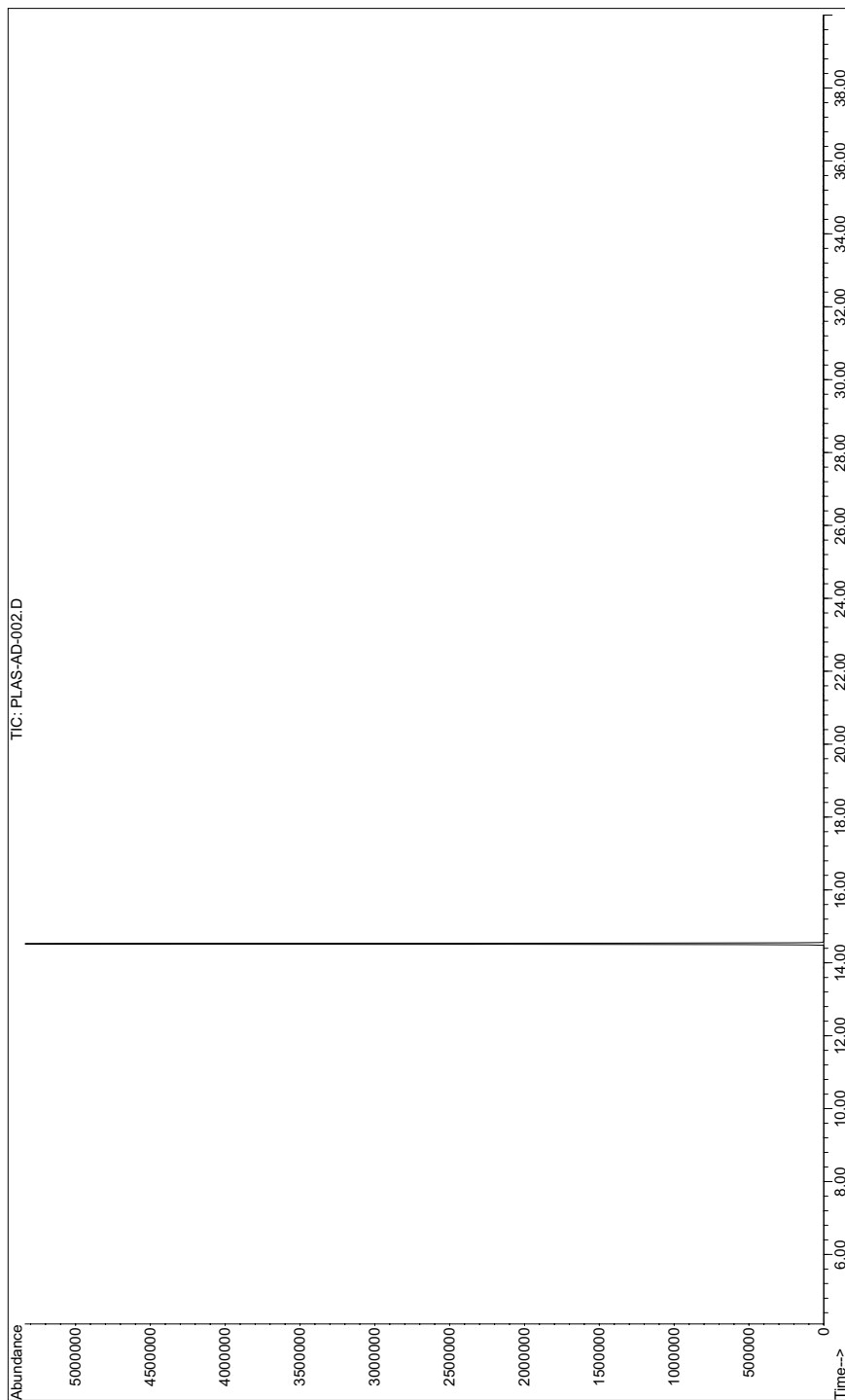
Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for 1,3-Diphenyl-2-thiourea - PLAS-AC-008****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for Dipentamethylenethiuram Tetrasulfide - PLAS-AC-009****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

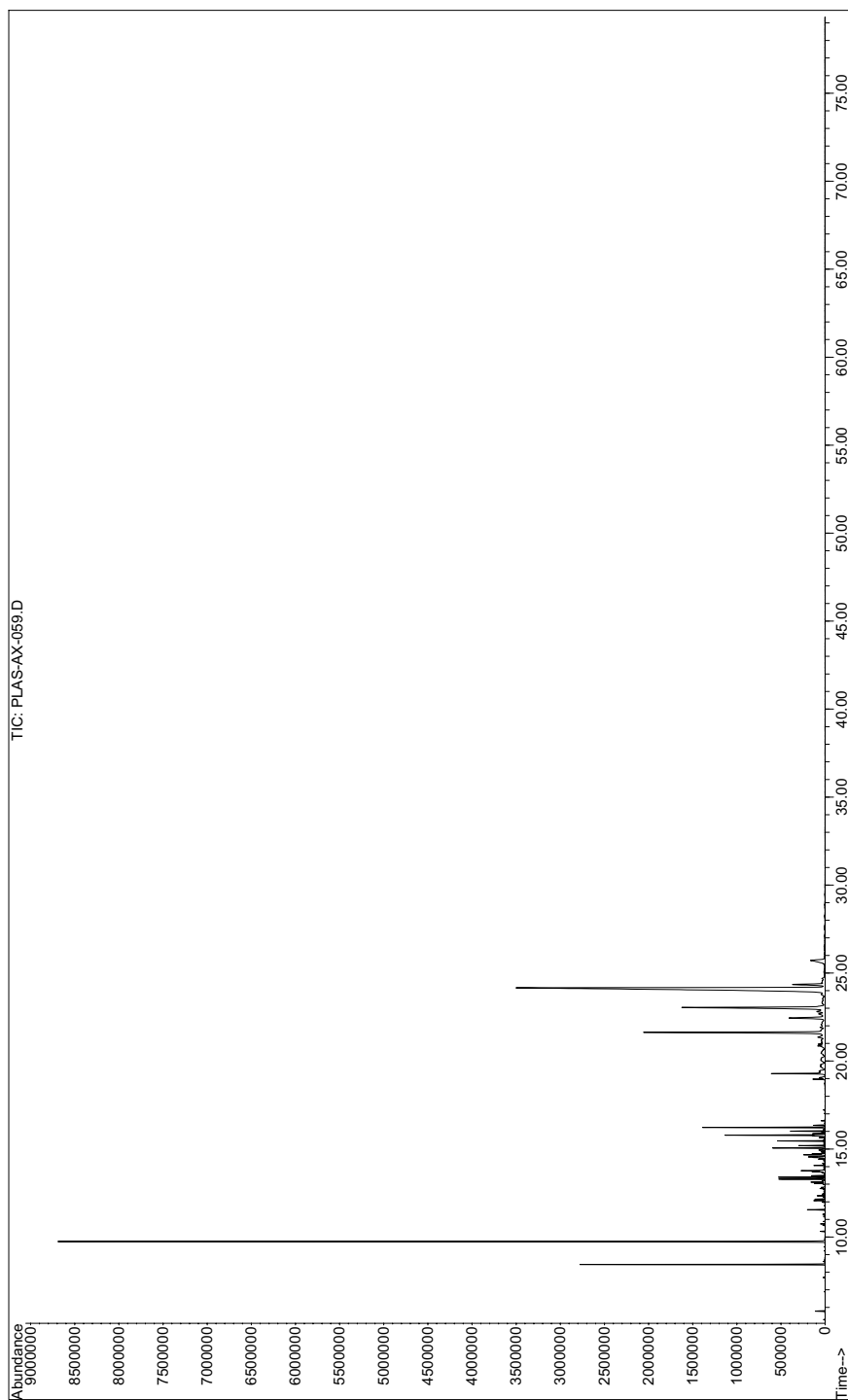
*Analytical Information***Chromatogram for 1,3-Di-o-tolylguanidine - PLAS-AC-010****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

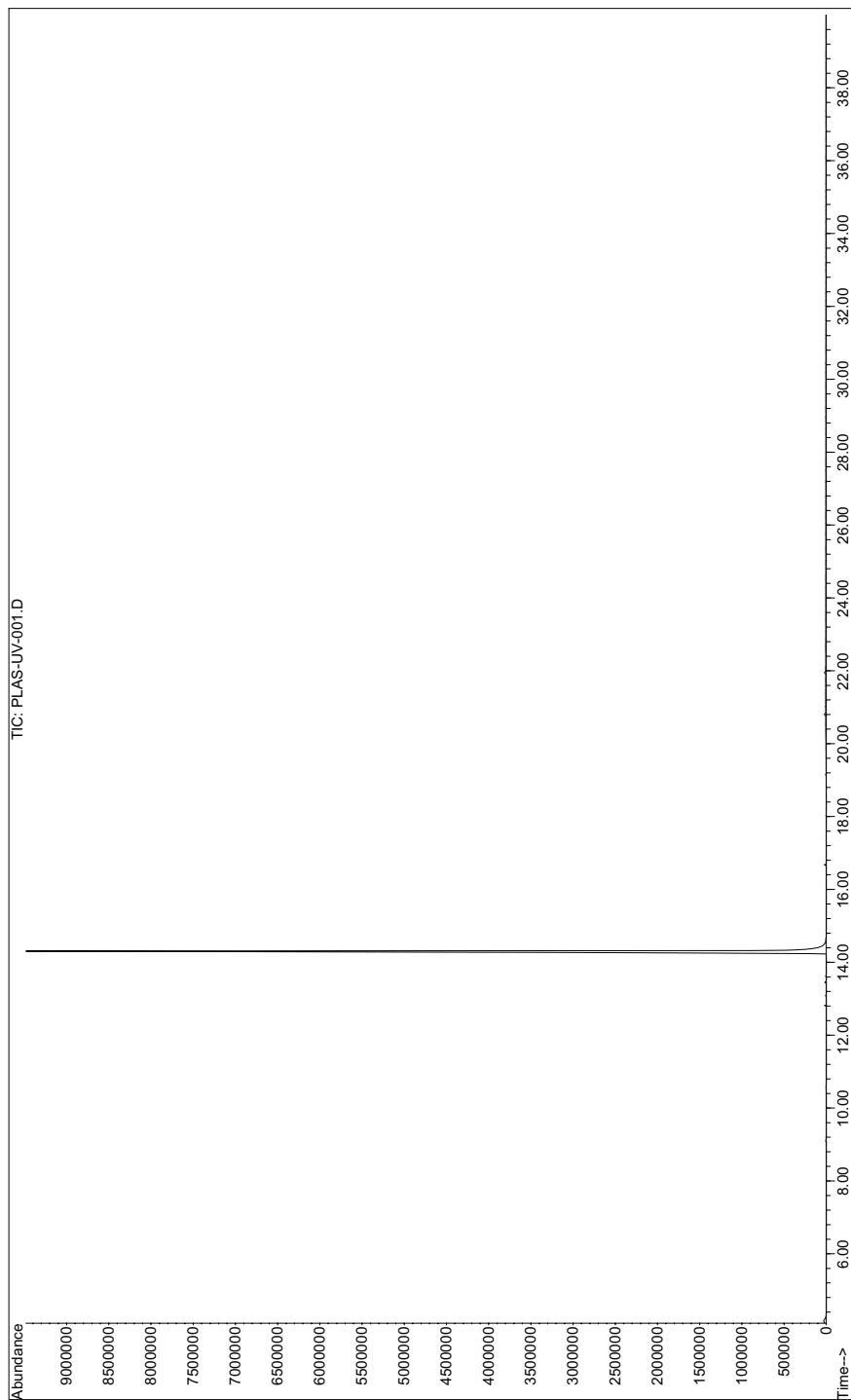
*Analytical Information***Chromatogram for *Santoflex*[®] 77PD - PLAS-AD-002****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

Analytical Information

Chromatogram for *Lowinox*[®] CPL - PLAS-AX-059

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

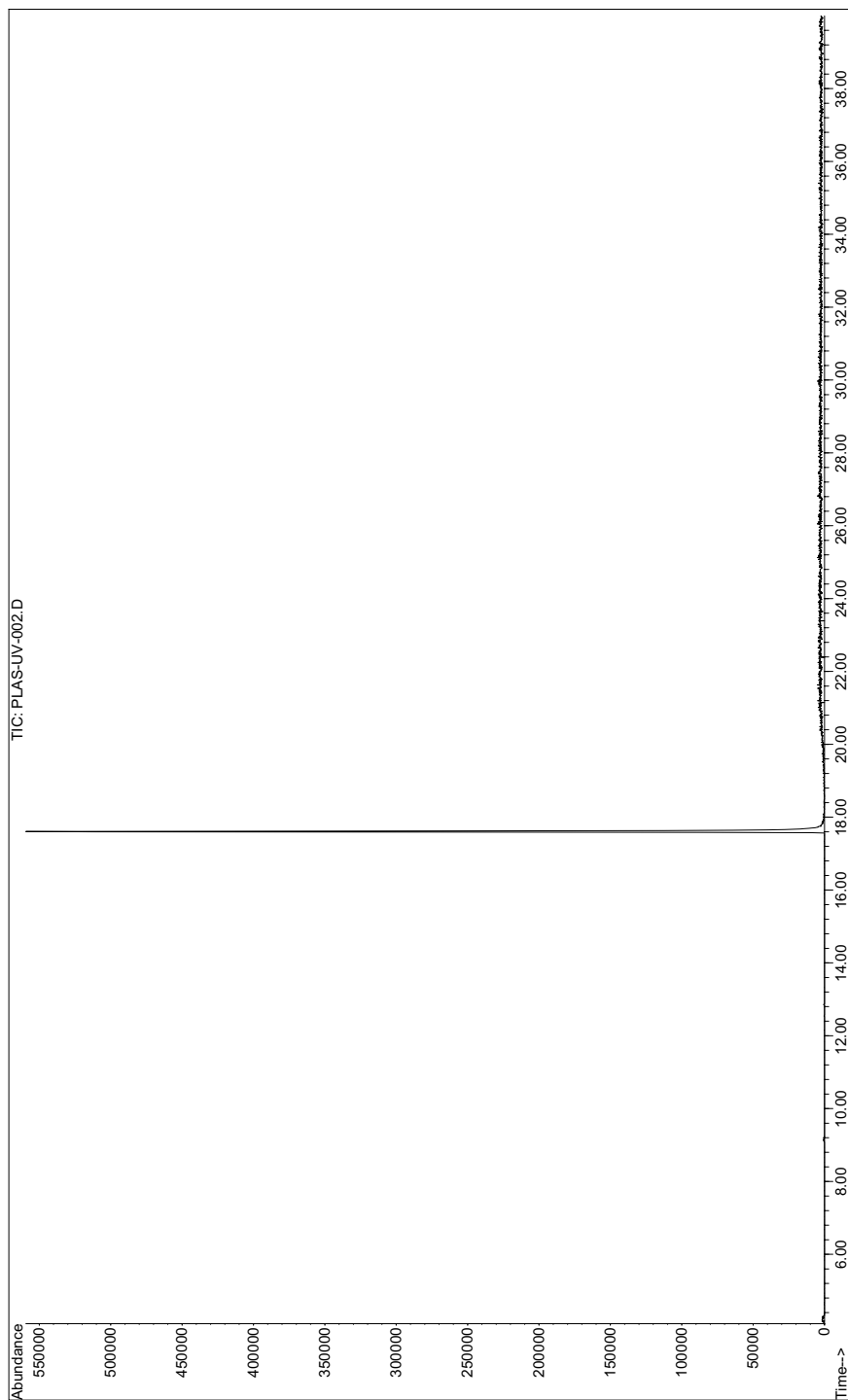


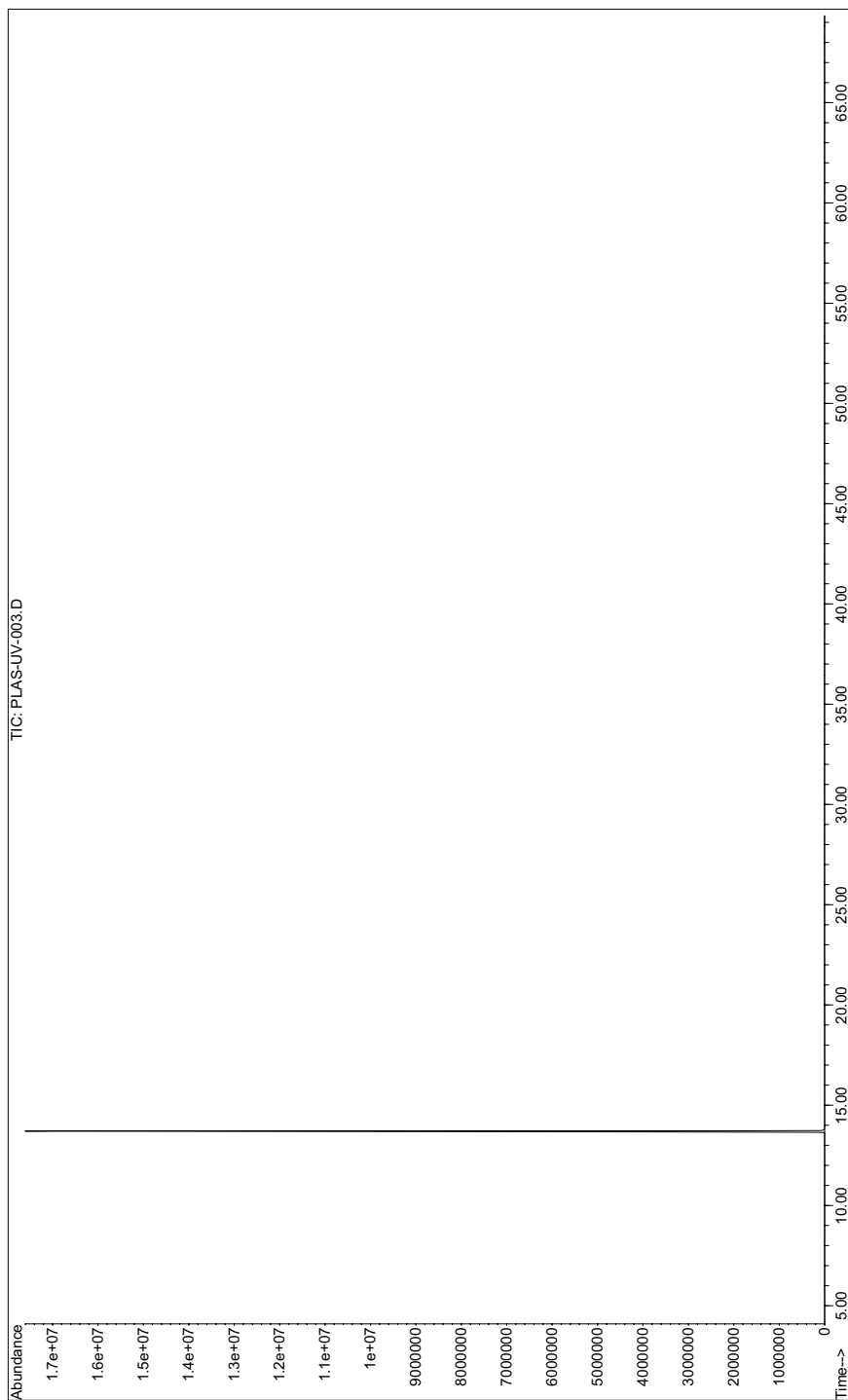
*Analytical Information***Chromatogram for Uvinul® 3000 - PLAS-UV-001****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

Analytical Information

Chromatogram for *Uvinul*[®] 3008 - PLAS-UV-002

Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

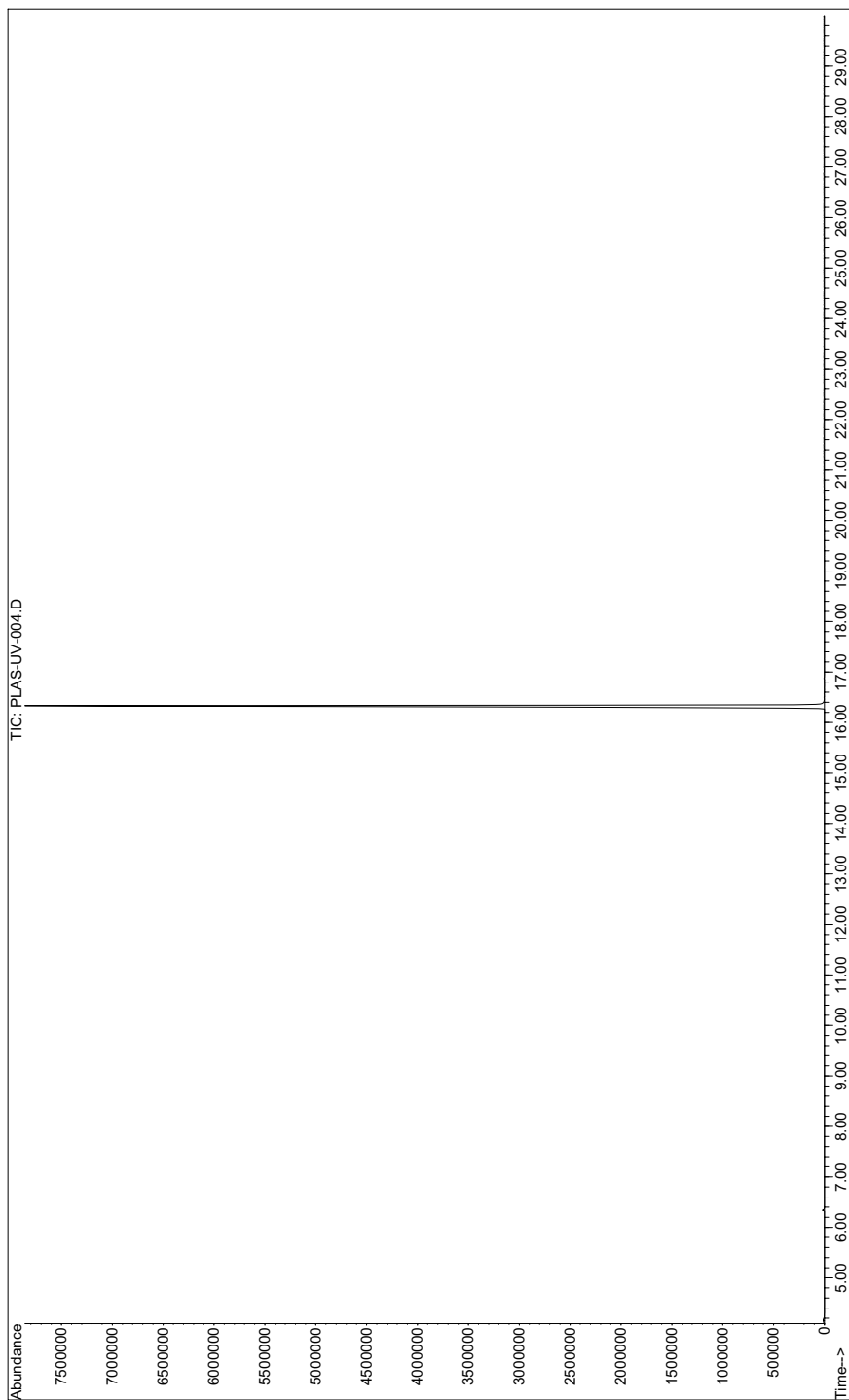


*Analytical Information***Chromatogram for Uvinul® 3040 - PLAS-UV-003****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

Analytical Information

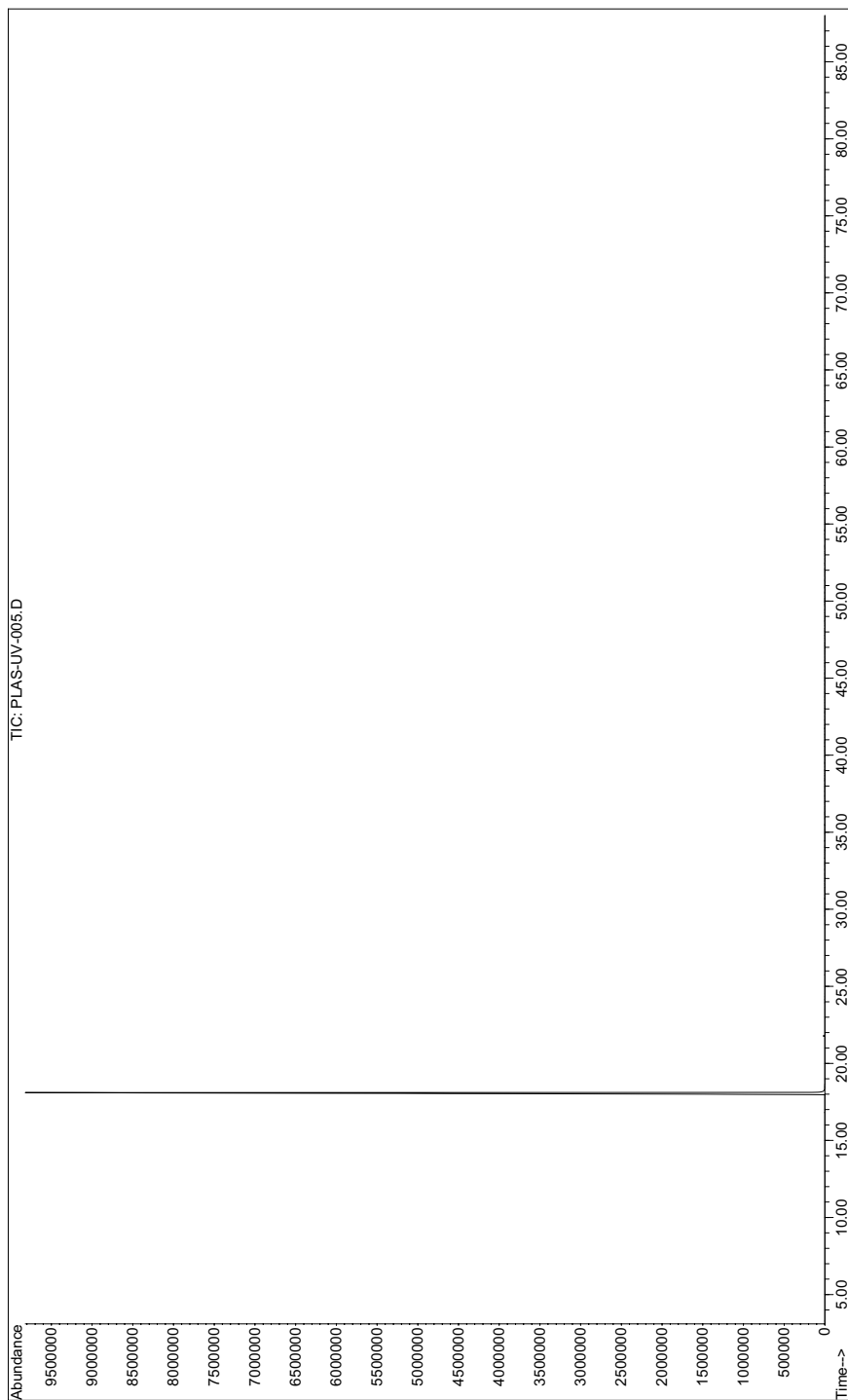
Chromatogram for *Uvinul*[®] 3049 - PLAS-UV-004

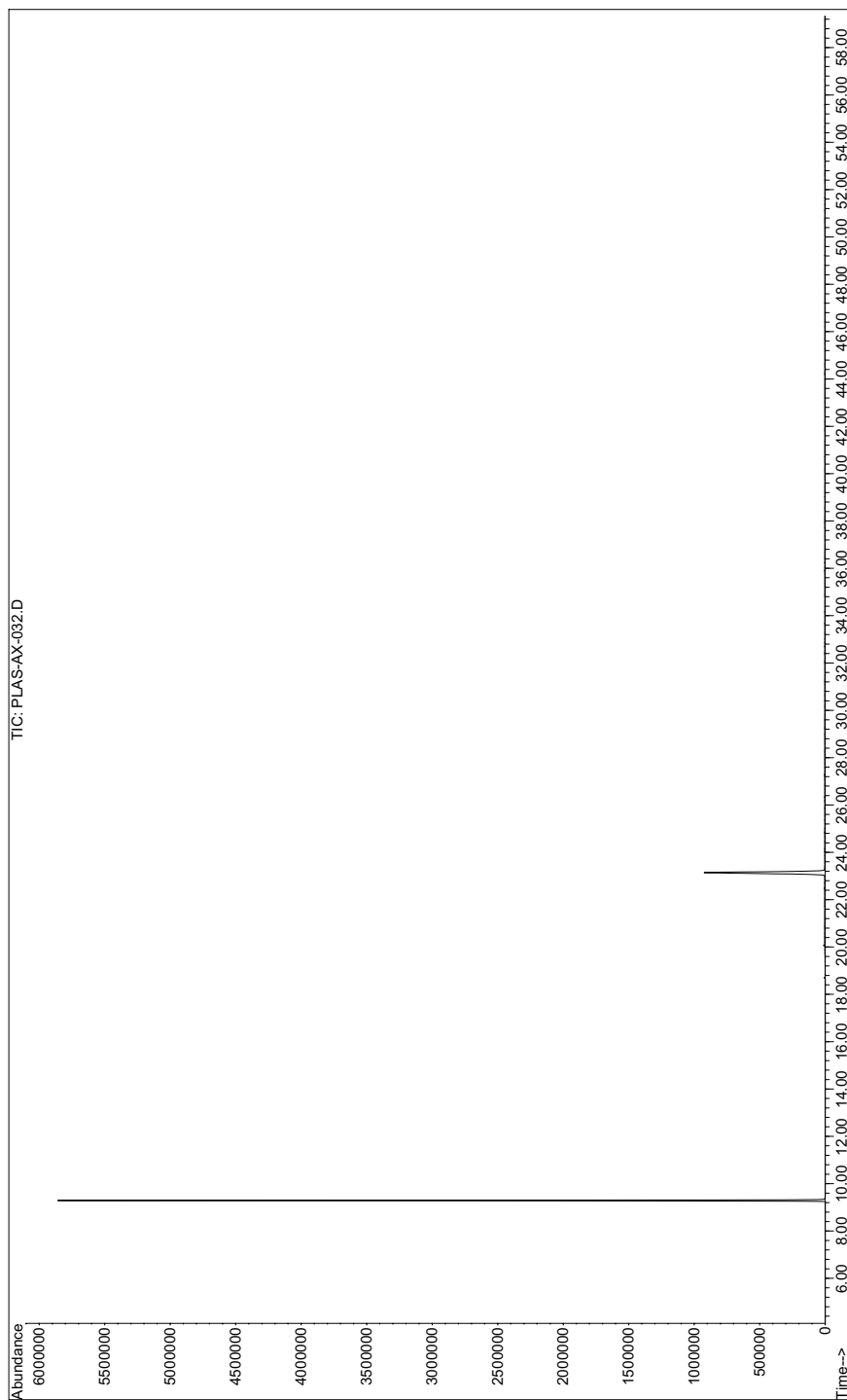
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



*Analytical Information***Chromatogram for *Tinuvin*[®] PED - PLAS-UV-005****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD

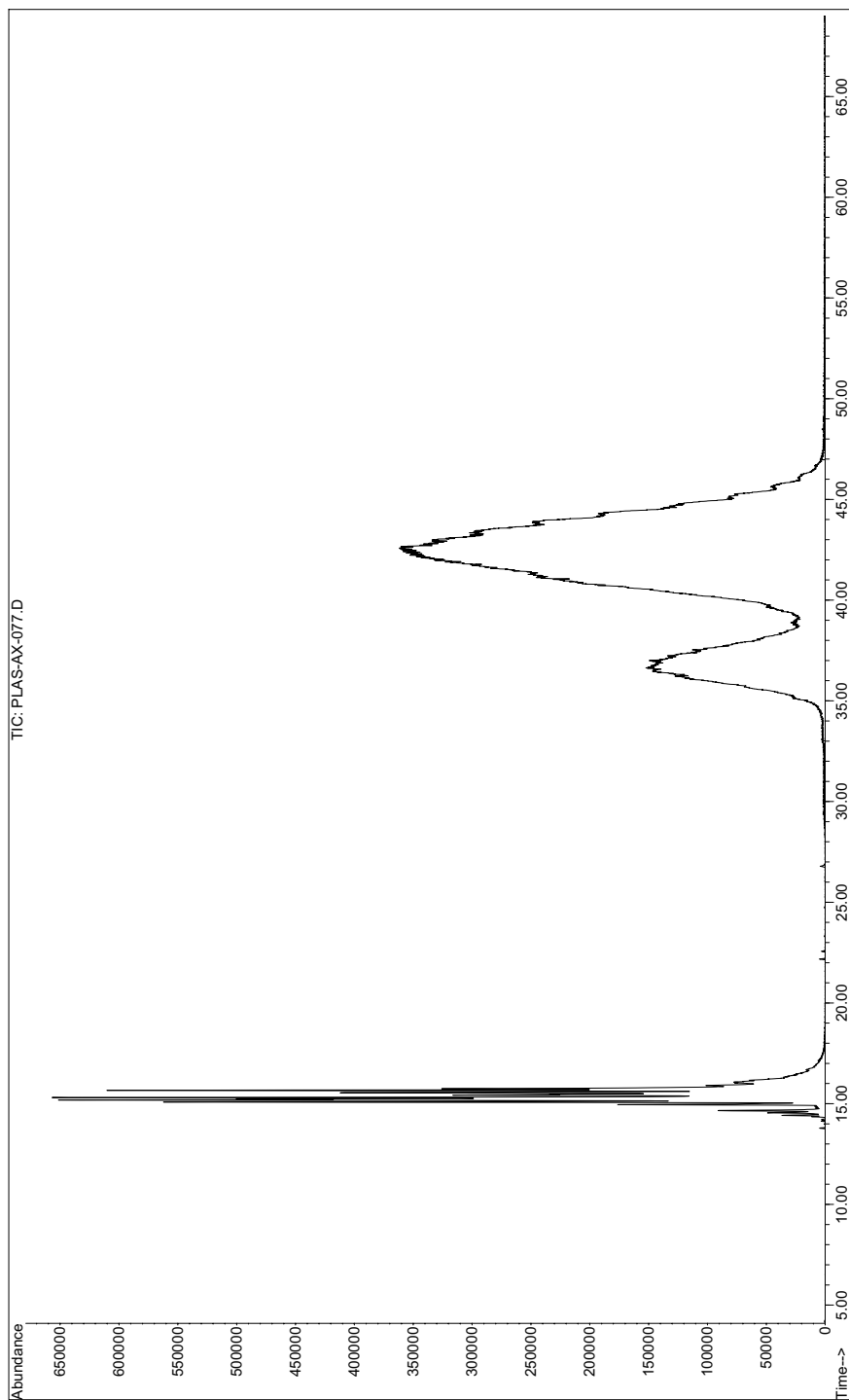


*Analytical Information***Chromatogram for *Alkanox*[®] P27 - PLAS-AX-032****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

Analytical Information

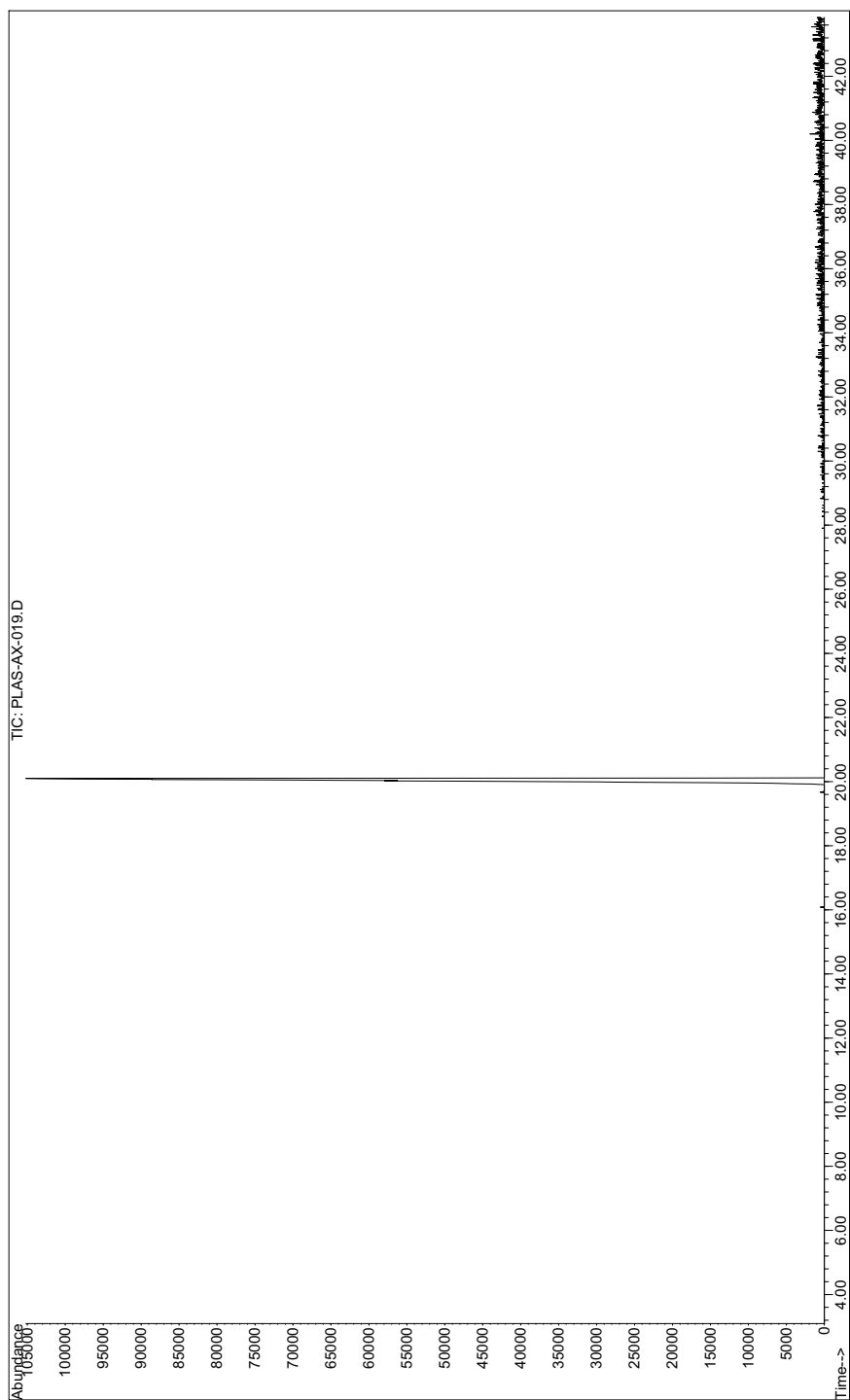
Chromatogram for *Alkanox*[®] TNPP - PLAS-AX-077

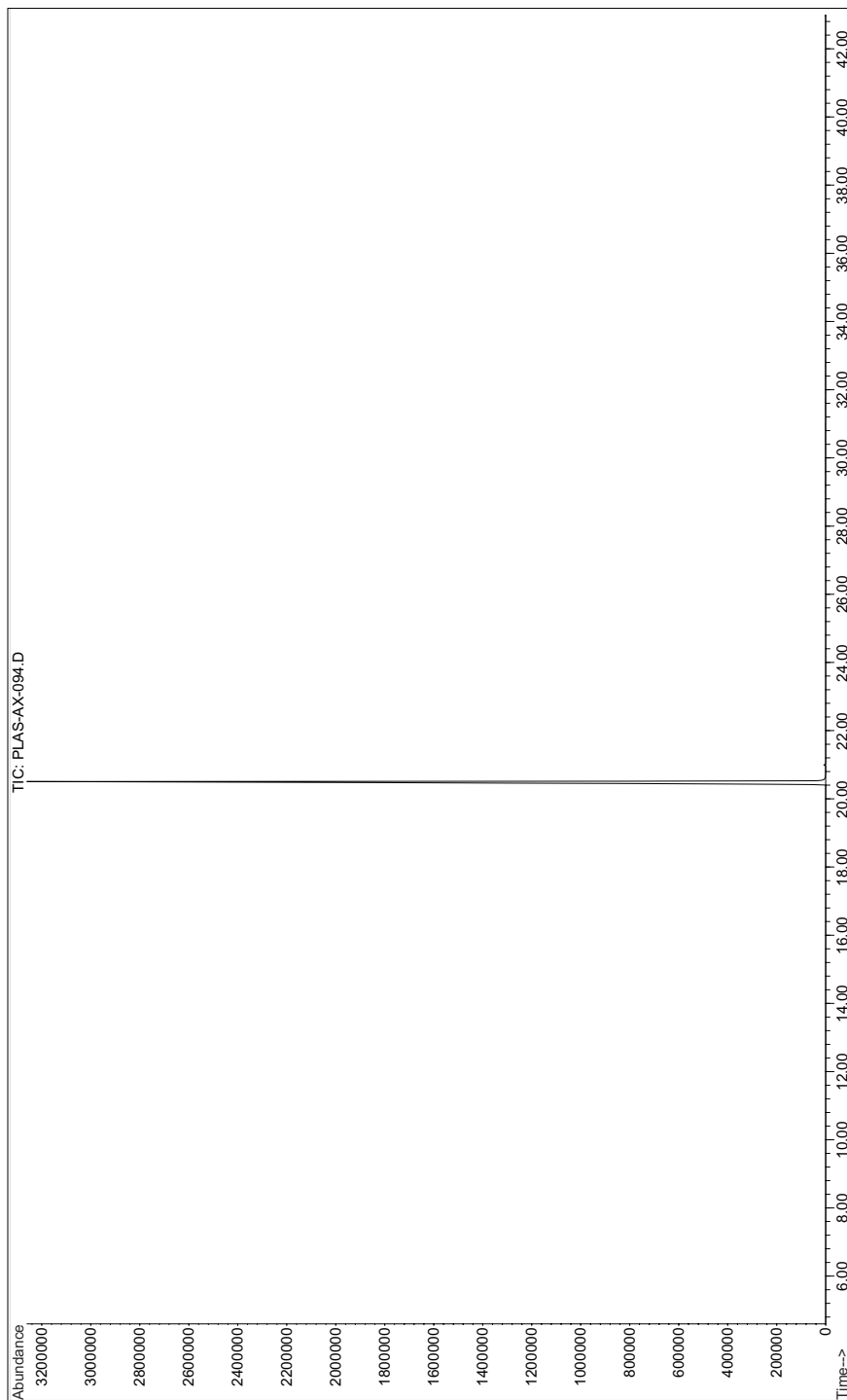
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



*Analytical Information***Chromatogram for *Antioxidant 60* - PLAS-AX-019****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD

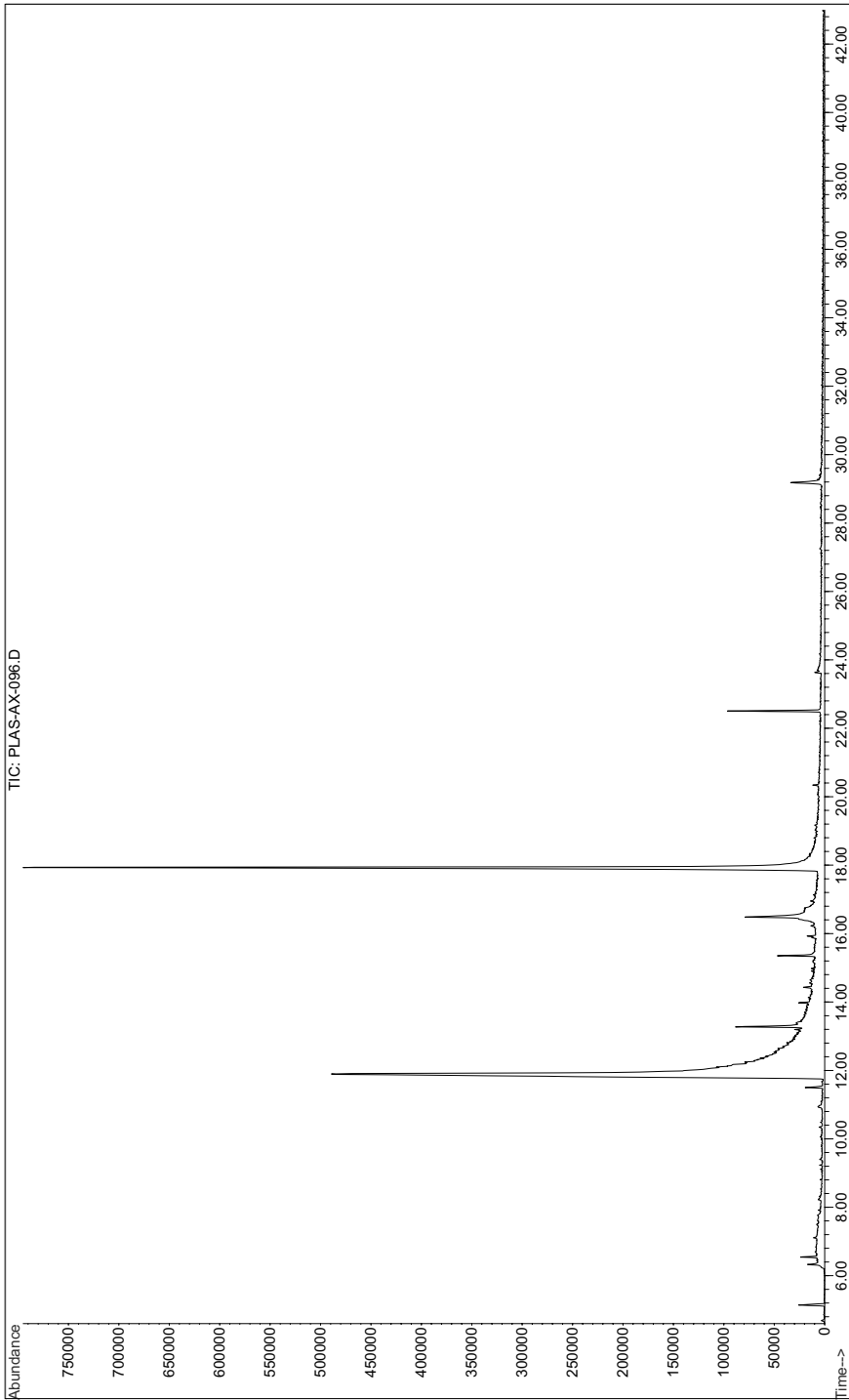


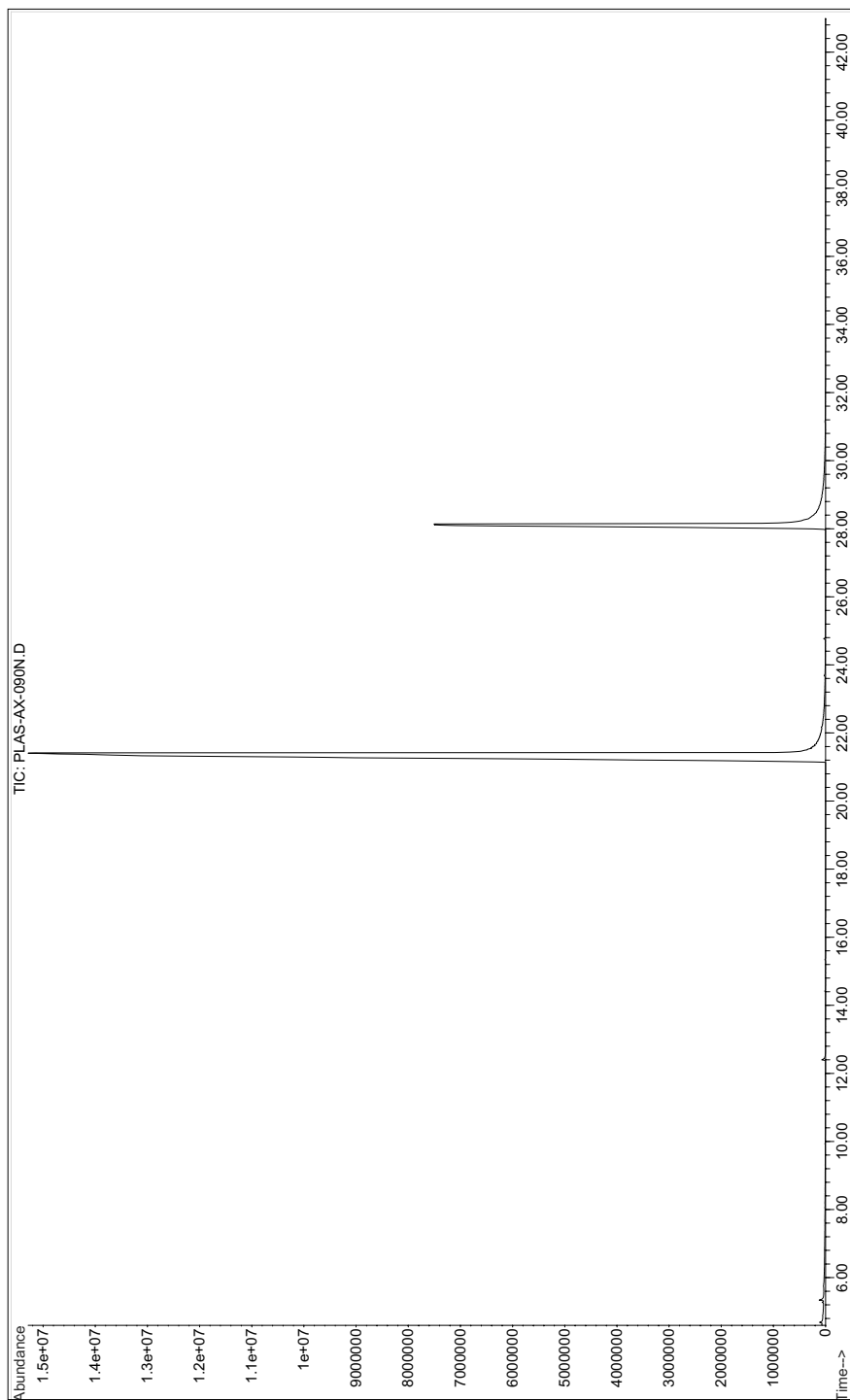
*Analytical Information***Chromatogram for 2-(2-Hydroxy-5-*t*-octylphenyl)benzotriazole - PLAS-AX-094****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *BLS 1622 - PLAS-AX-096*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

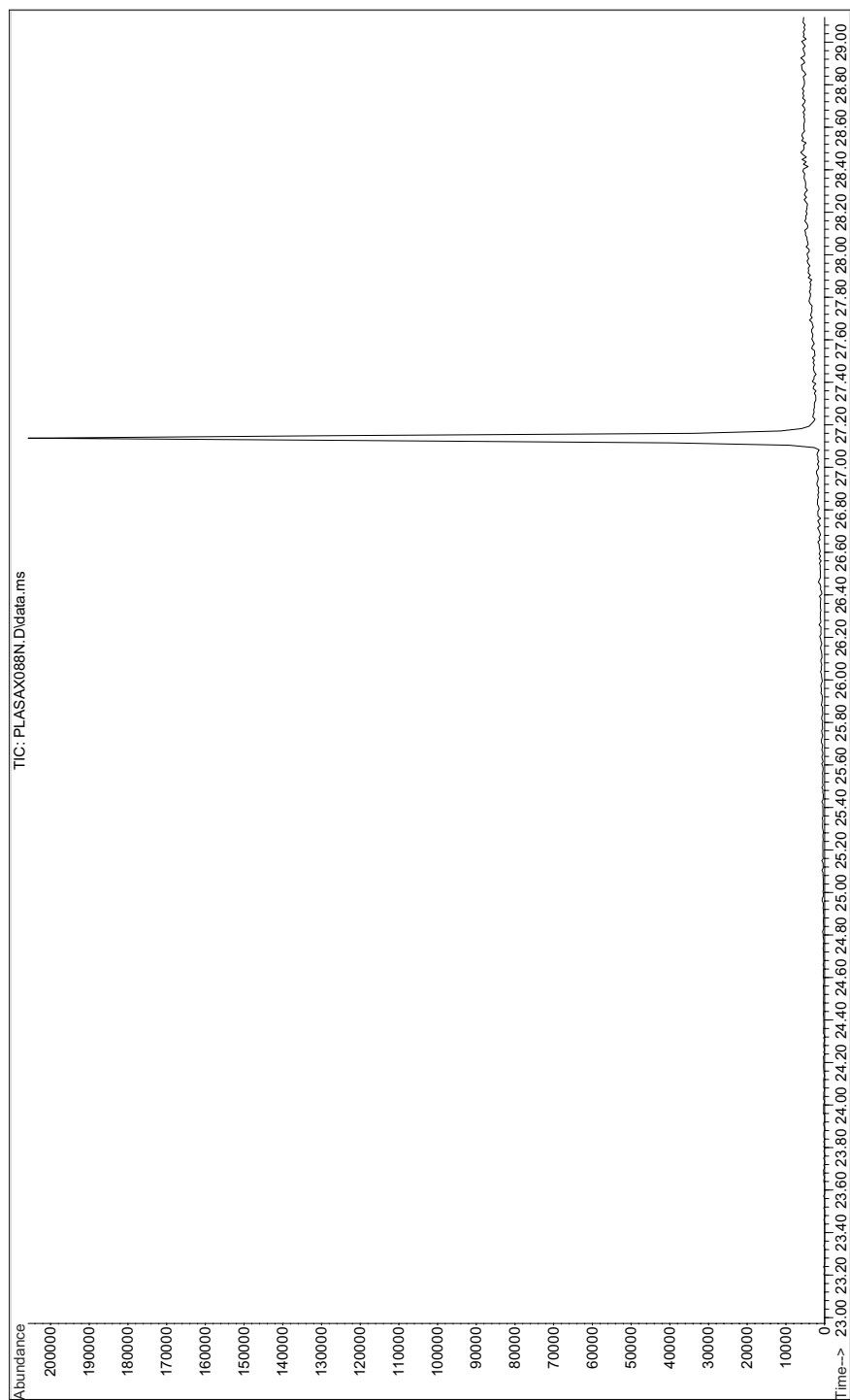


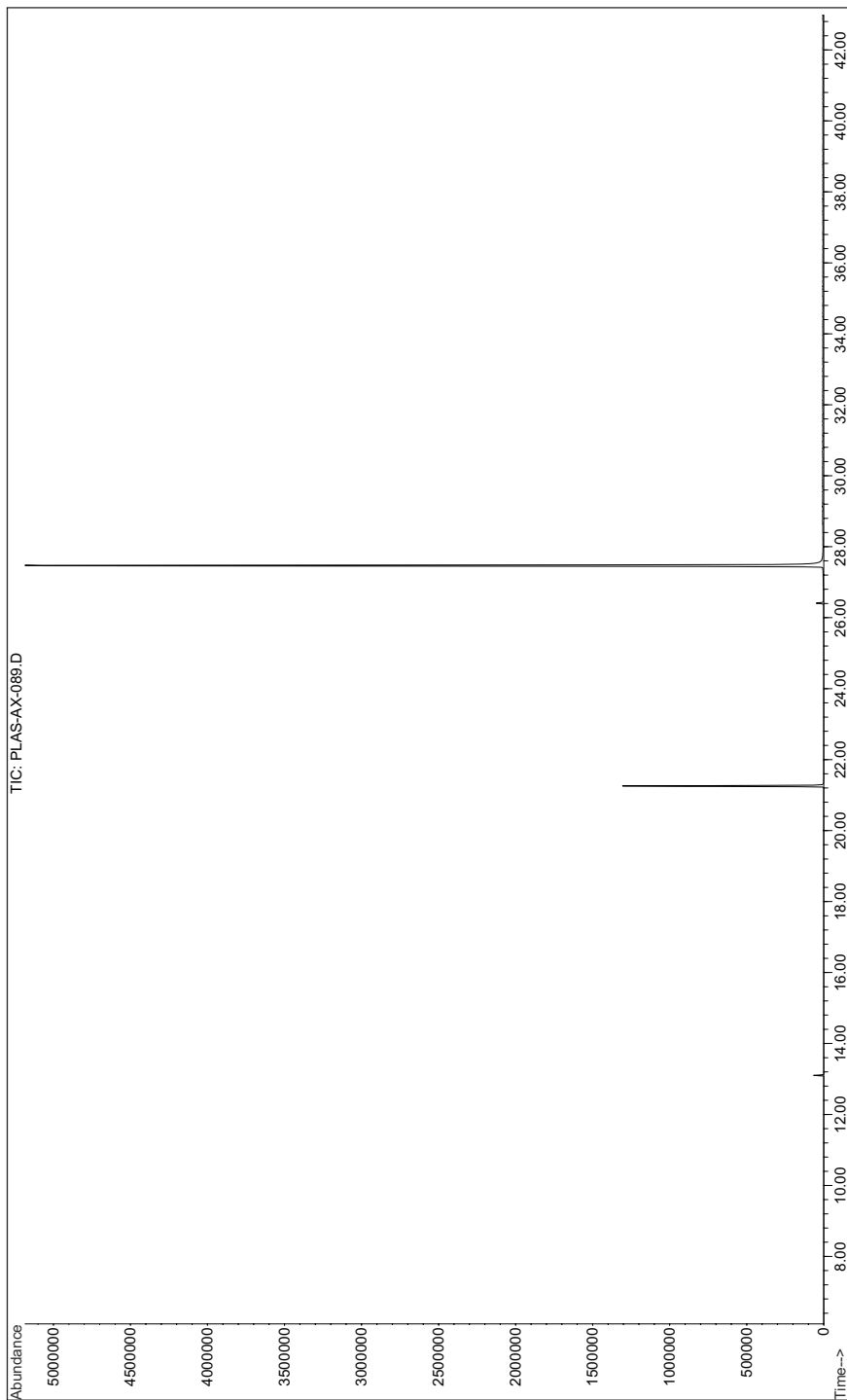
*Analytical Information***Chromatogram for BLS-1944 - PLAS-AX-090****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *BLS 234 - PLAS-AX-088*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

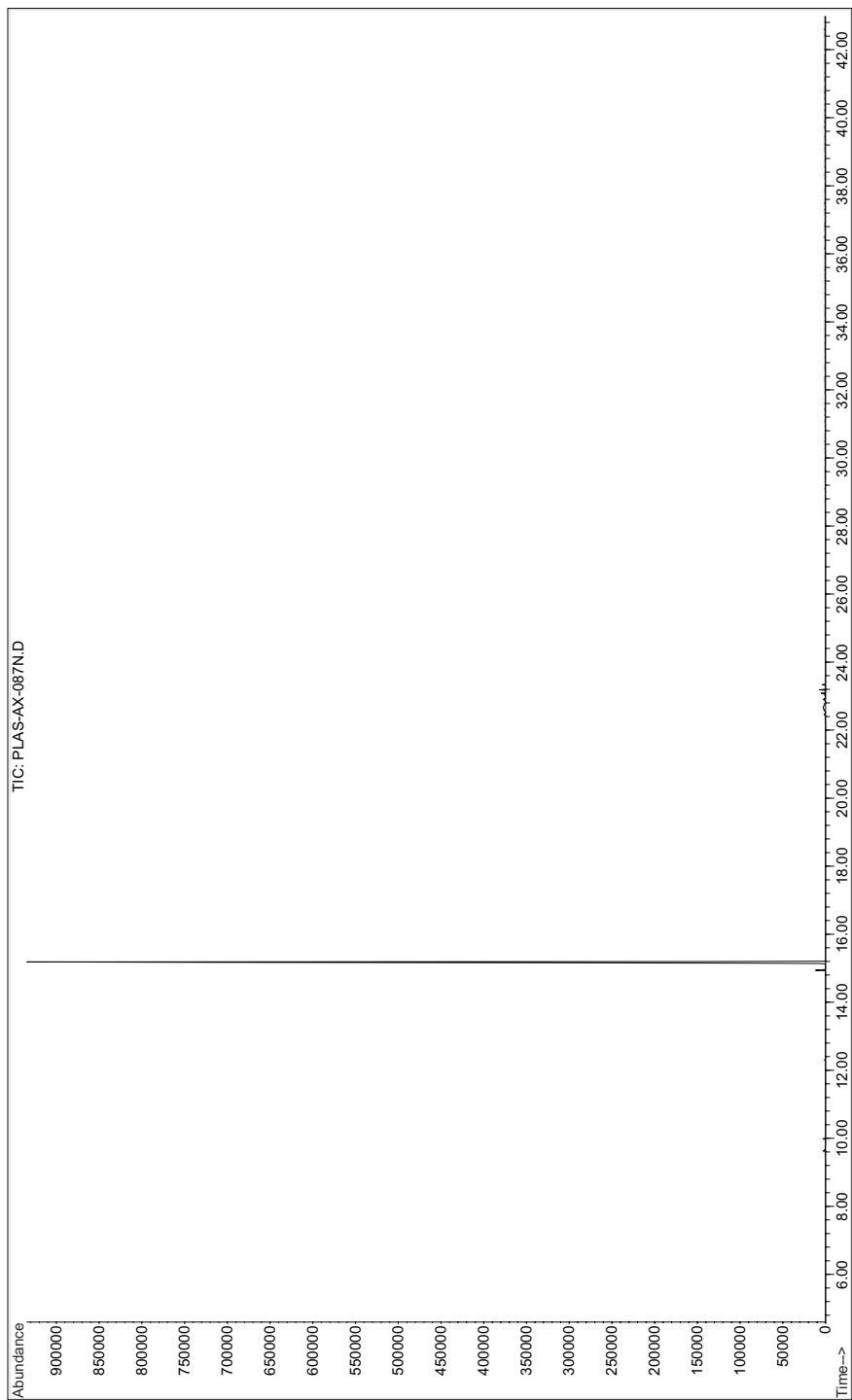


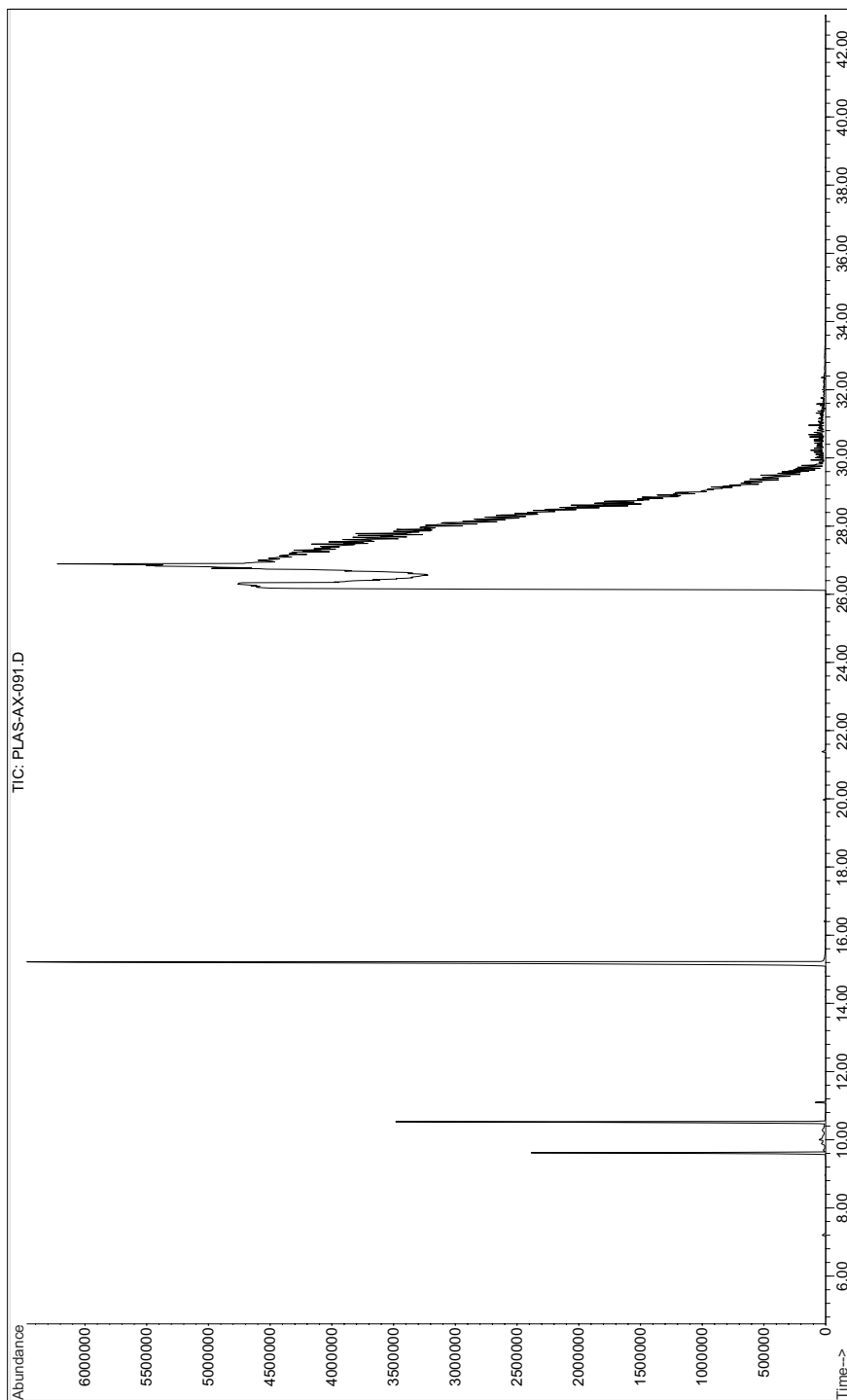
*Analytical Information***Chromatogram for BLS 292 - PLAS-AX-089****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

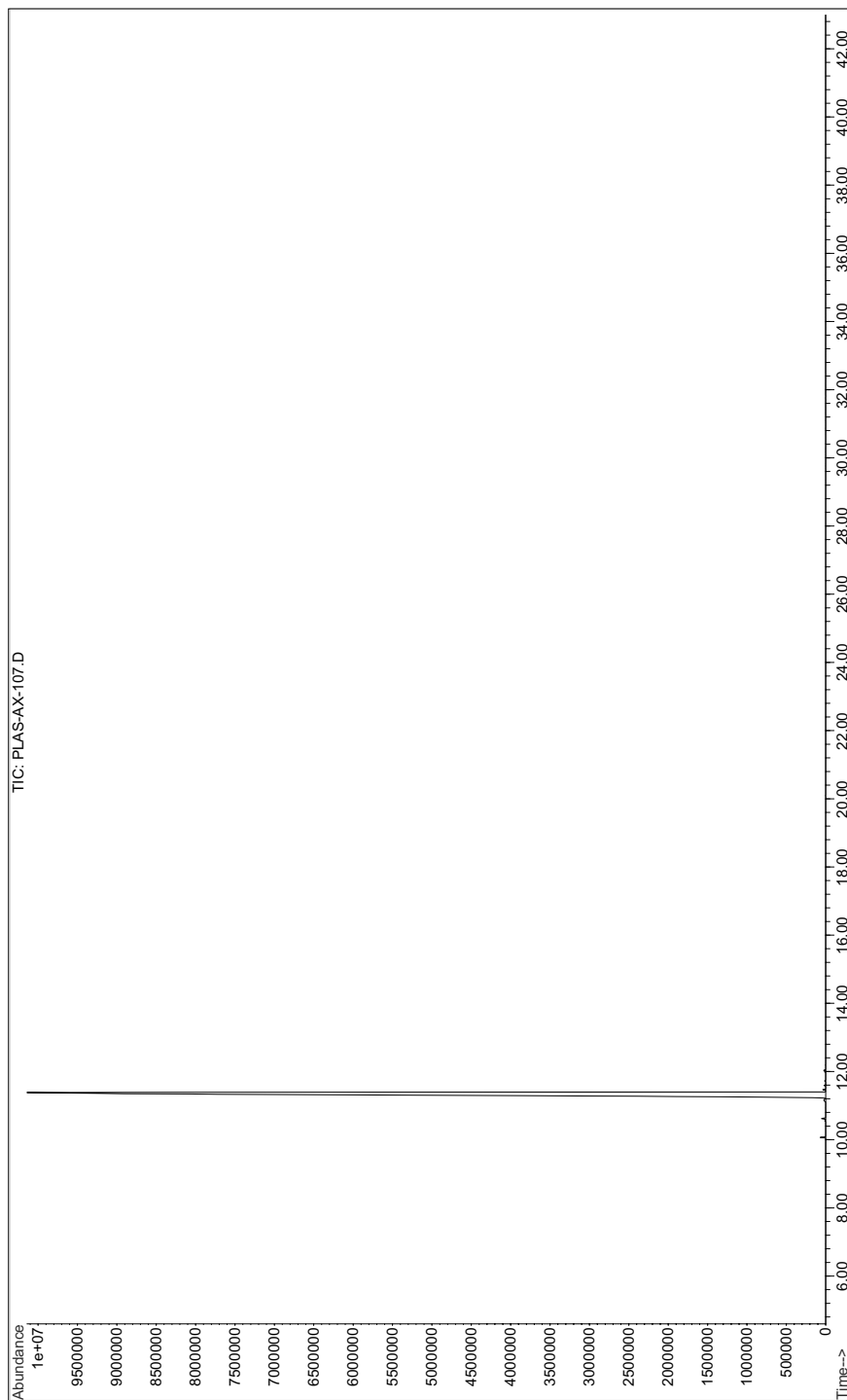
Analytical Information

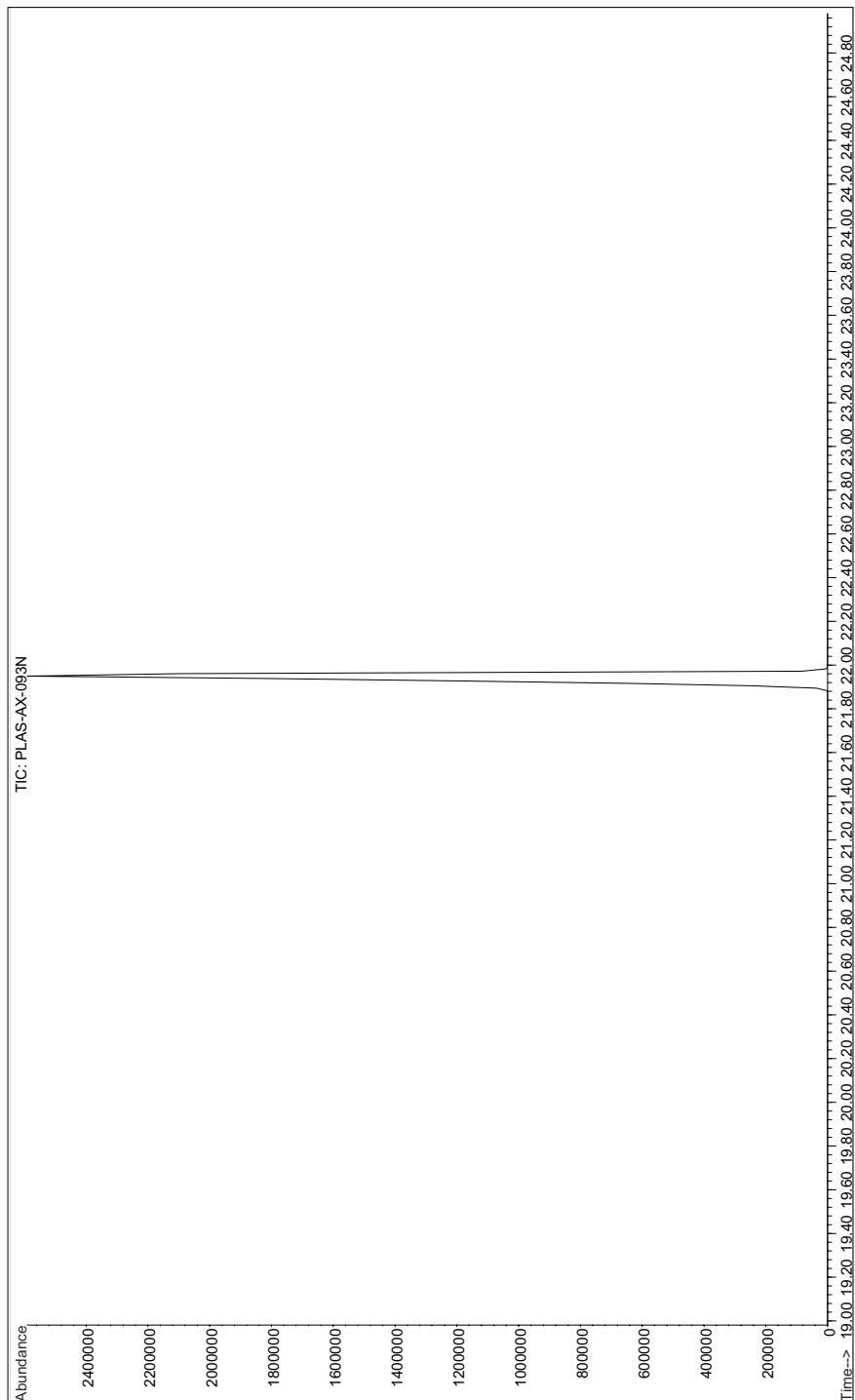
Chromatogram for *BNX 1077 - PLAS-AX-087*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *BNX 1225 - PLAS-AX-091*****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

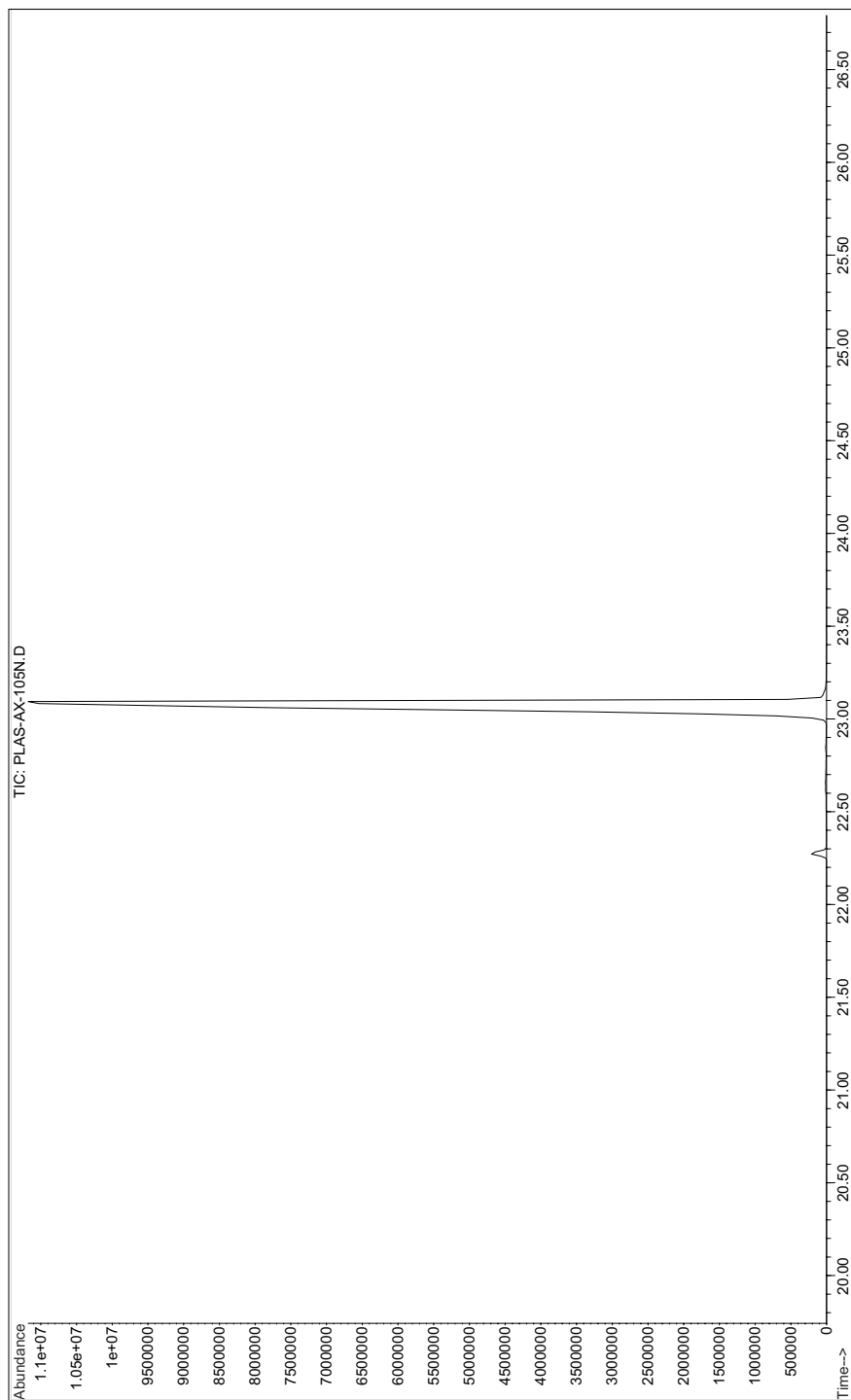
*Analytical Information***Chromatogram for 2,6-Di-tert-butyl-4-ethylphenol - PLAS-AX-107****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

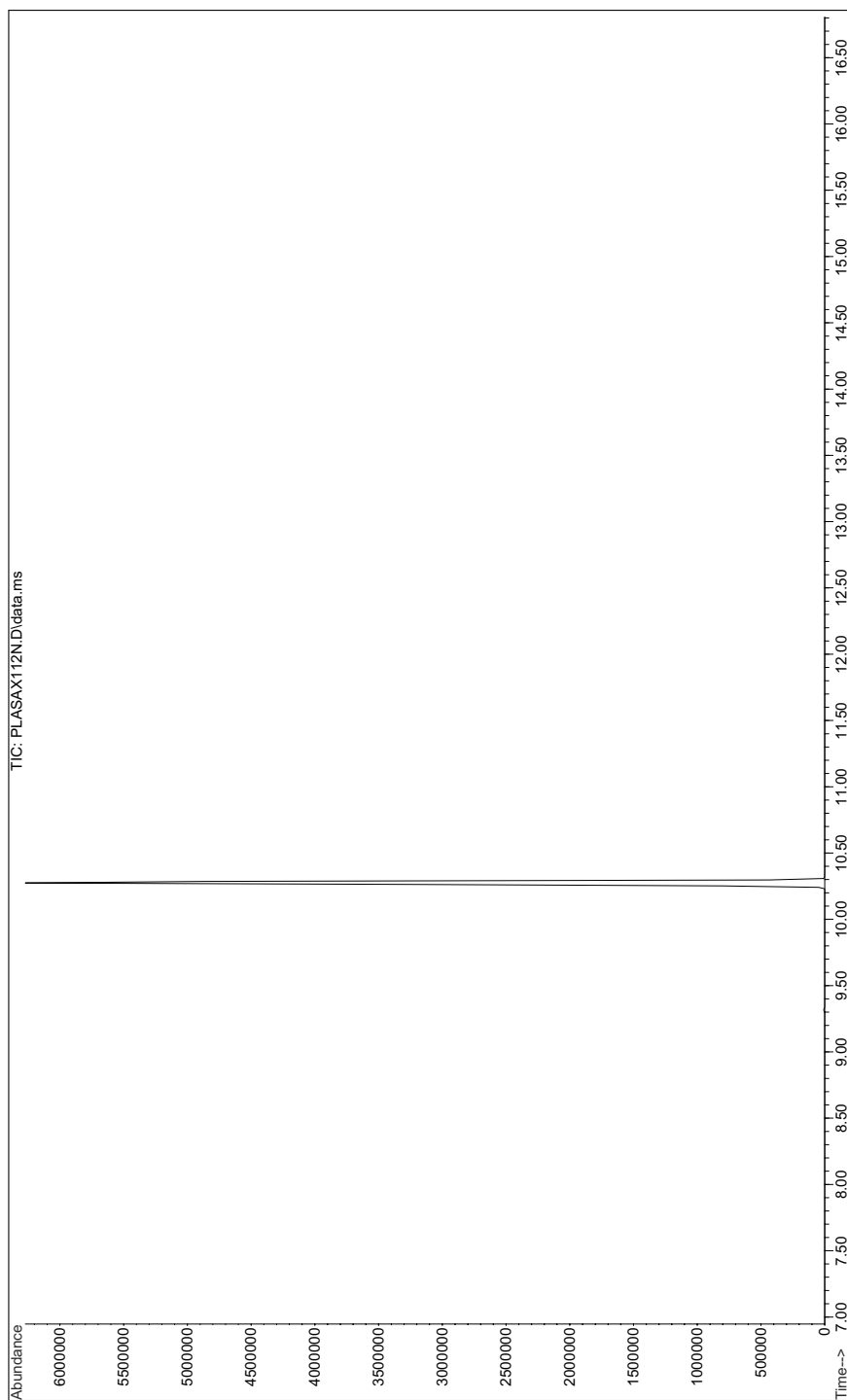
*Analytical Information***Chromatogram for 2-tert-butyl-6-(5-chlorobenzotriazol-2-yl)-4-methylphenol - PLAS-AX-093****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for 4,4'-Butylidenebis(6-tert-butyl-m-cresol) - PLAS-AX-105

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

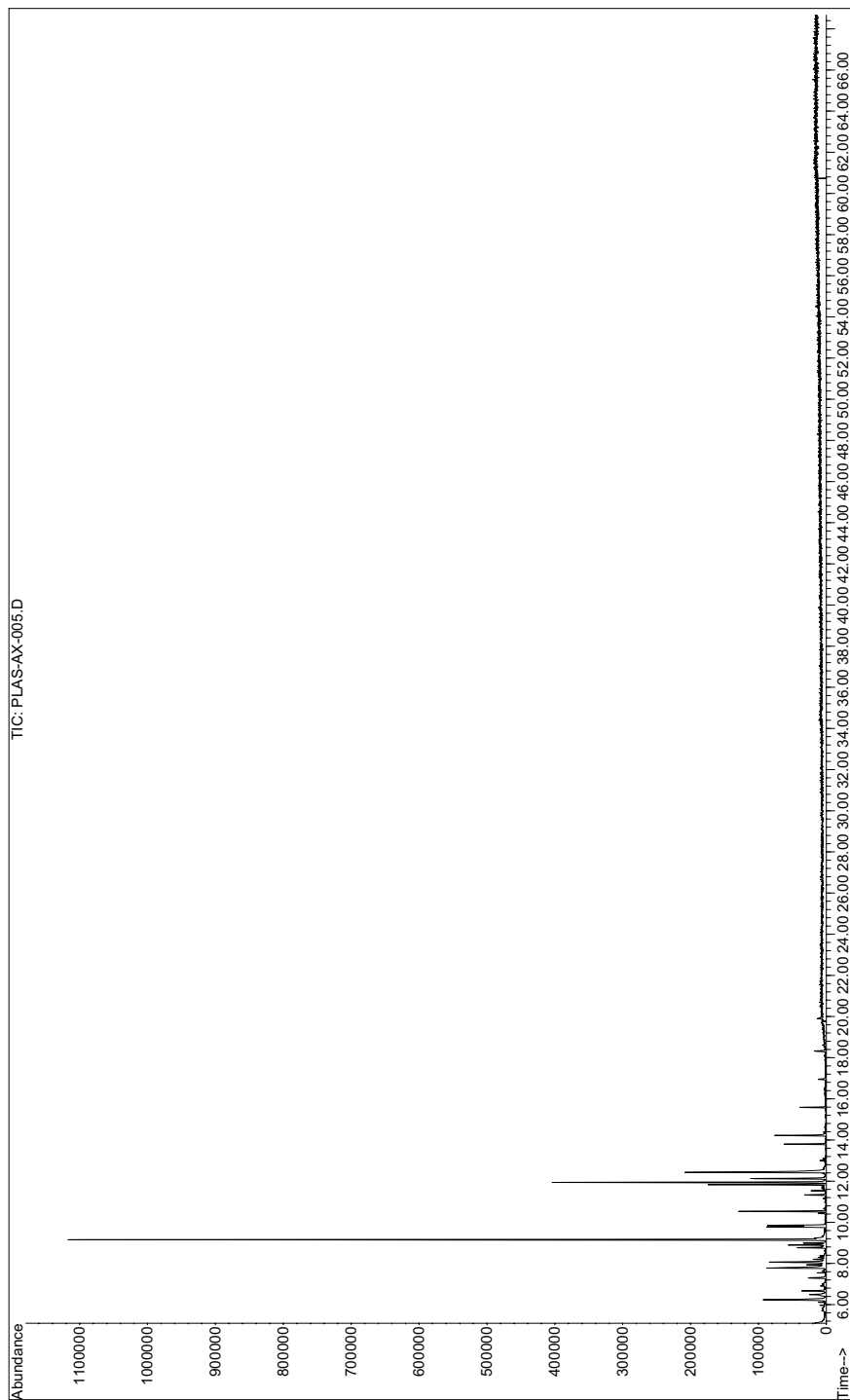


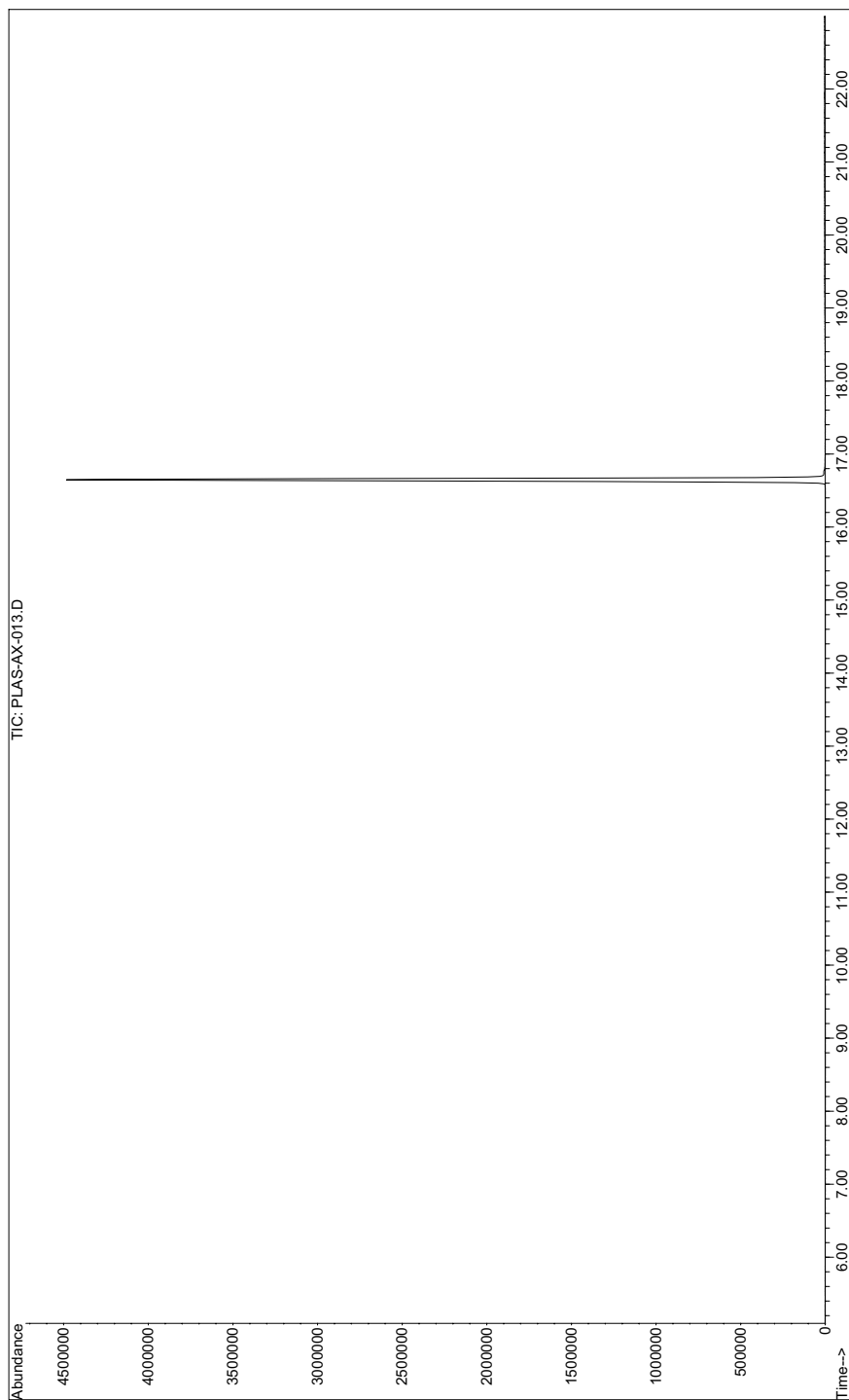
*Analytical Information***Chromatogram for 2,6-Di-*tert*-butylphenol - PLAS-AX-112****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *Cyanox[®] 1790 - PLAS-AX-005*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

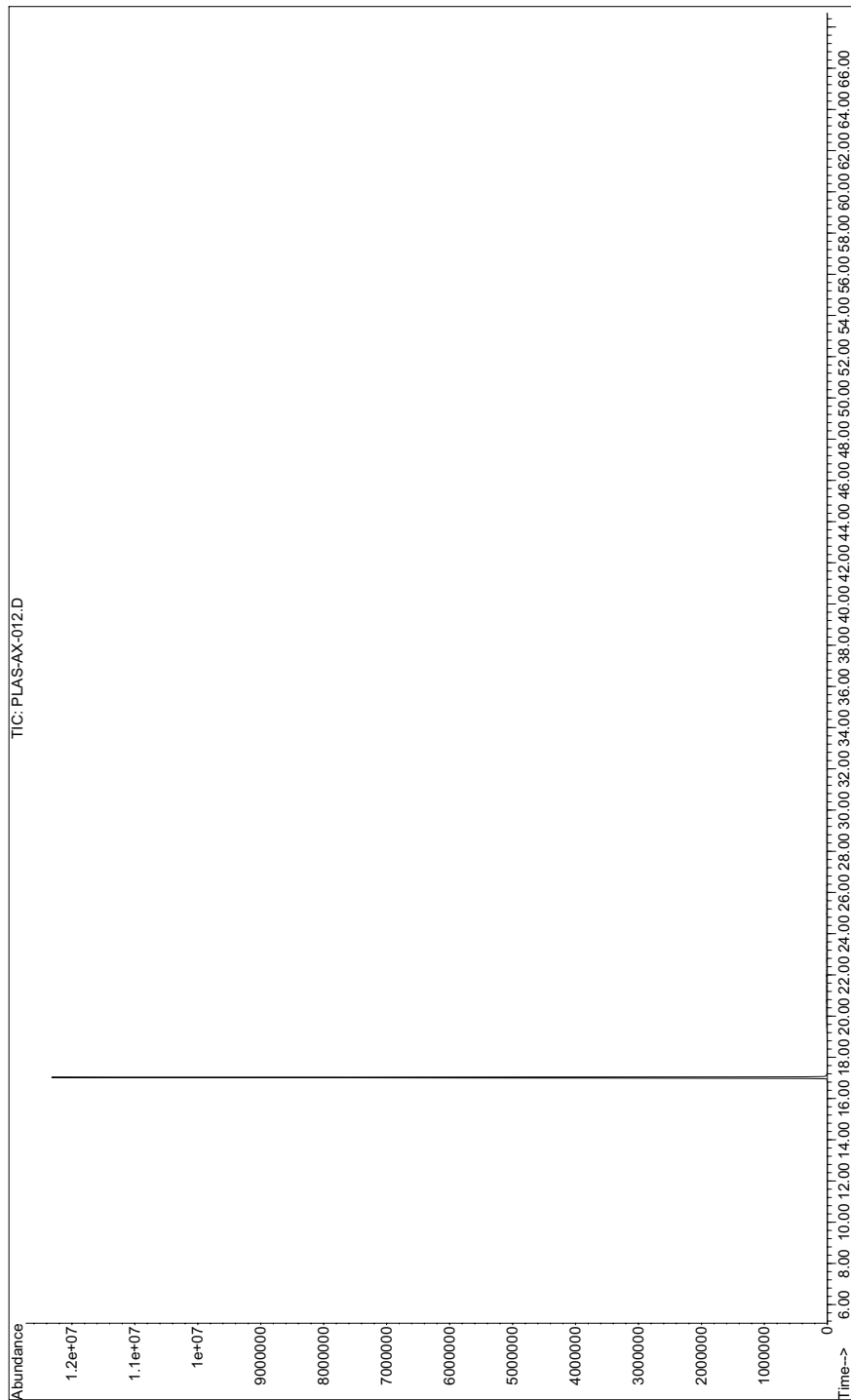


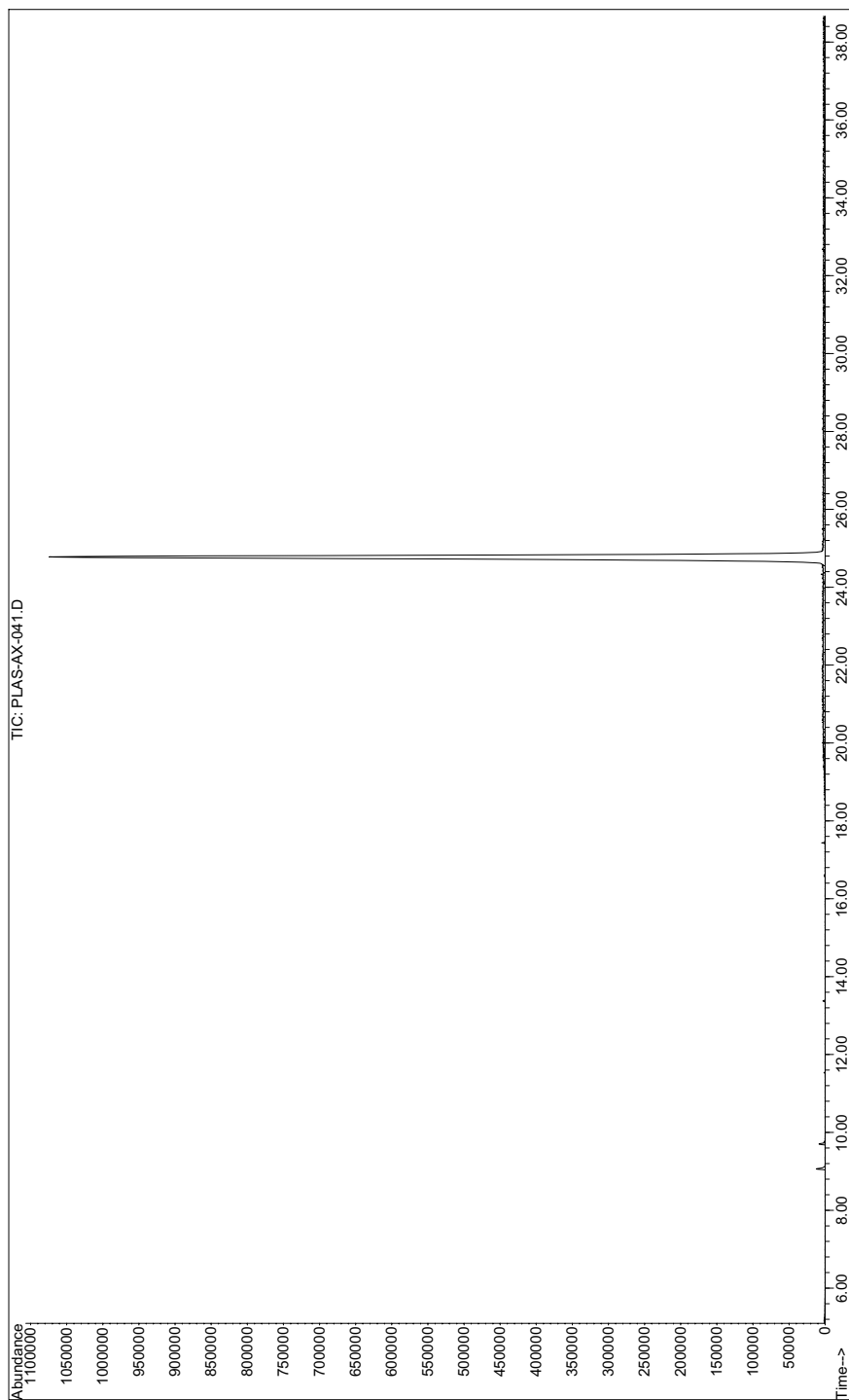
*Analytical Information***Chromatogram for *Cyanox*[®] 2246 - PLAS-AX-013****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

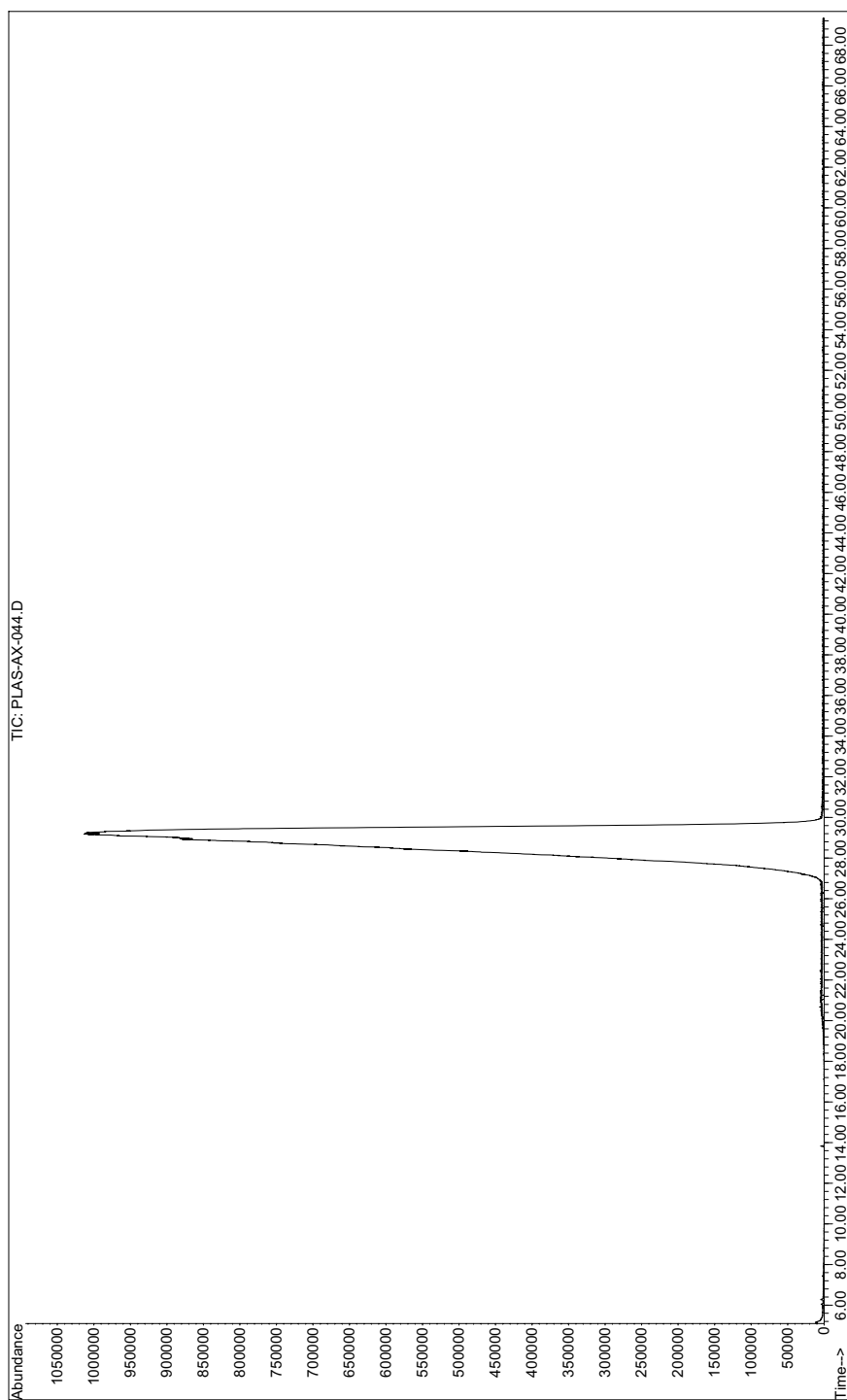
Analytical Information

Chromatogram for *Cyanox[®] 425 - PLAS-AX-012*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



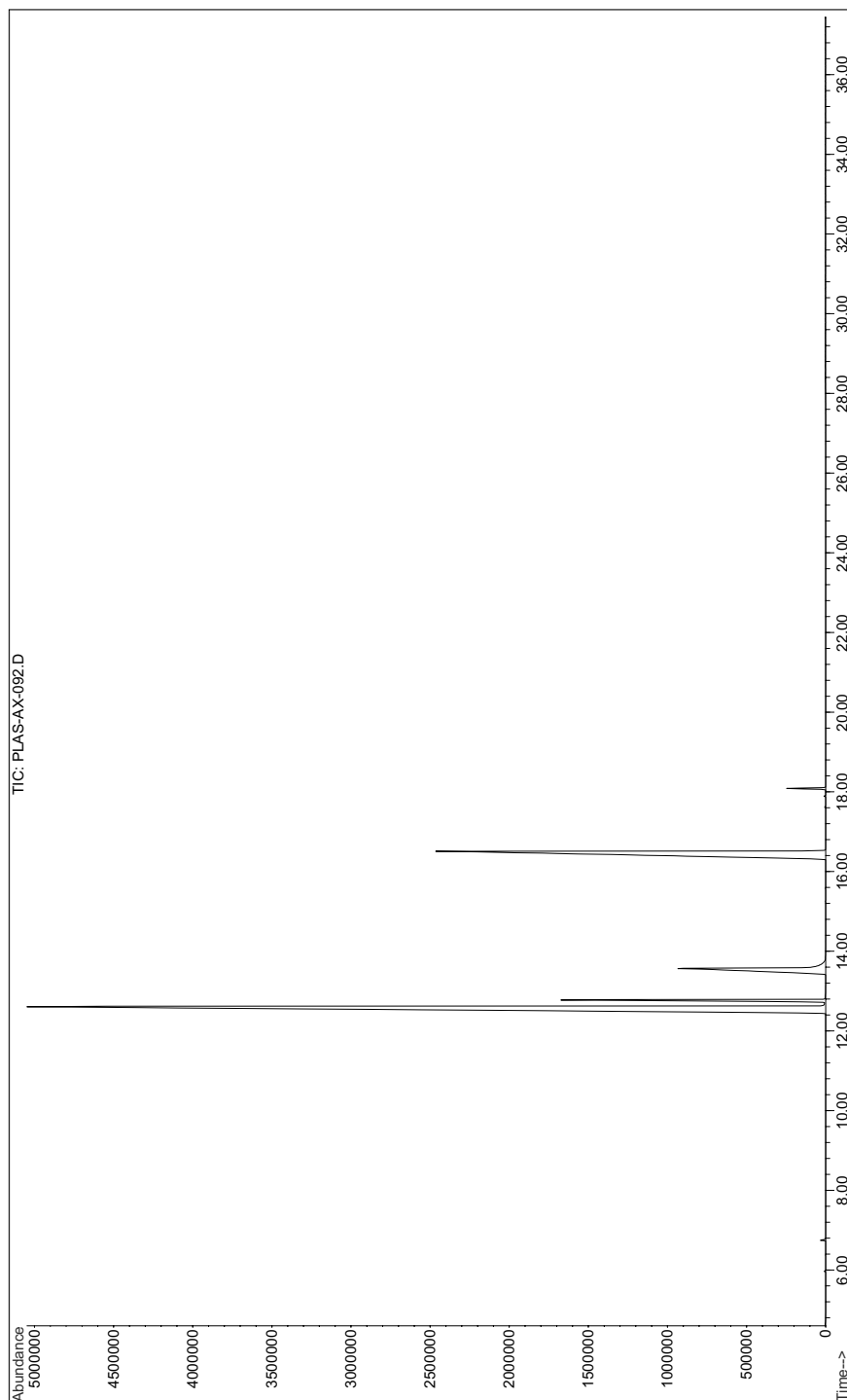
*Analytical Information***Chromatogram for *Cyanox*[®] LTDP - PLAS-AX-041****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

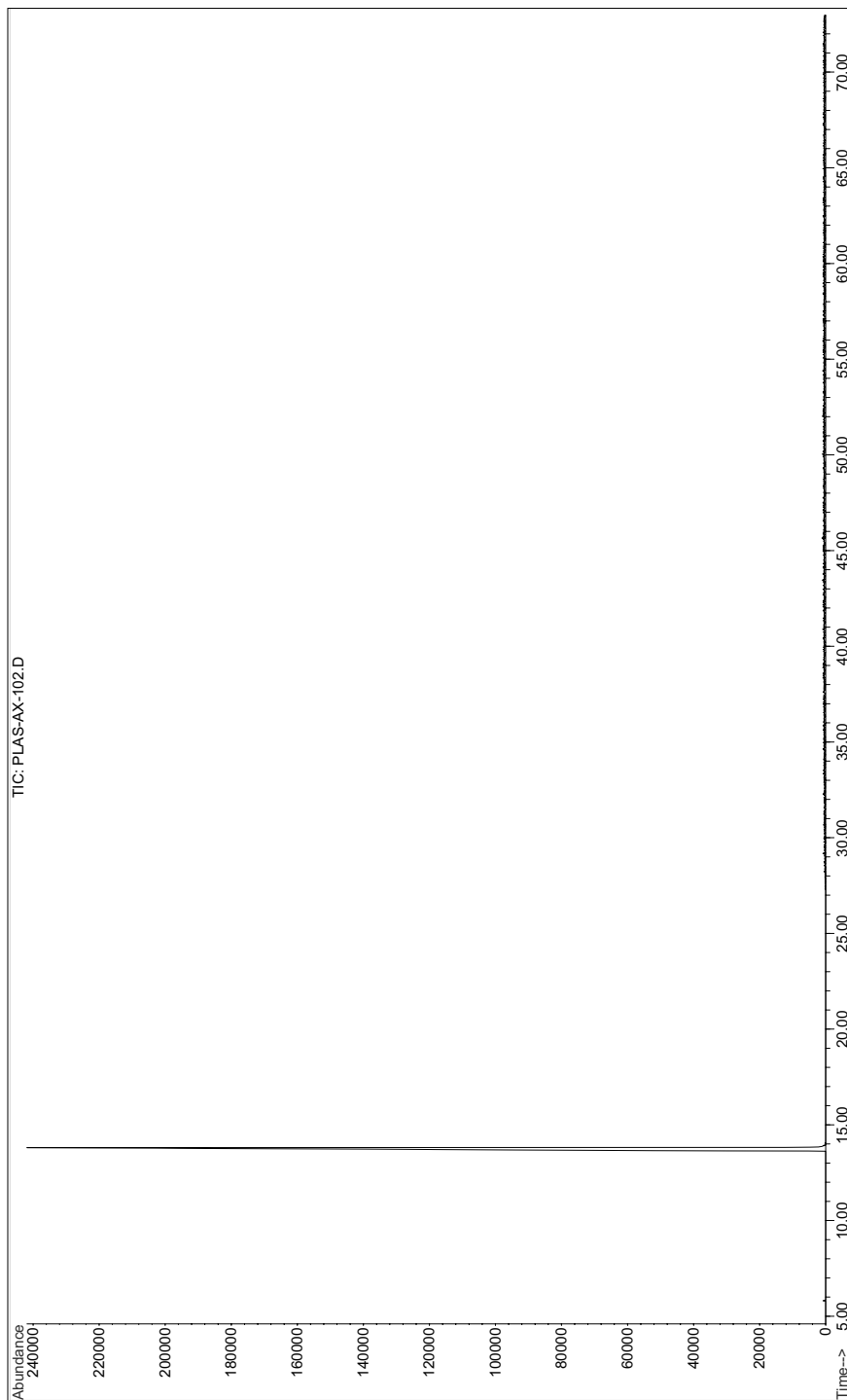
*Analytical Information***Chromatogram for Cyanox[®] STDP - PLAS-AX-044****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

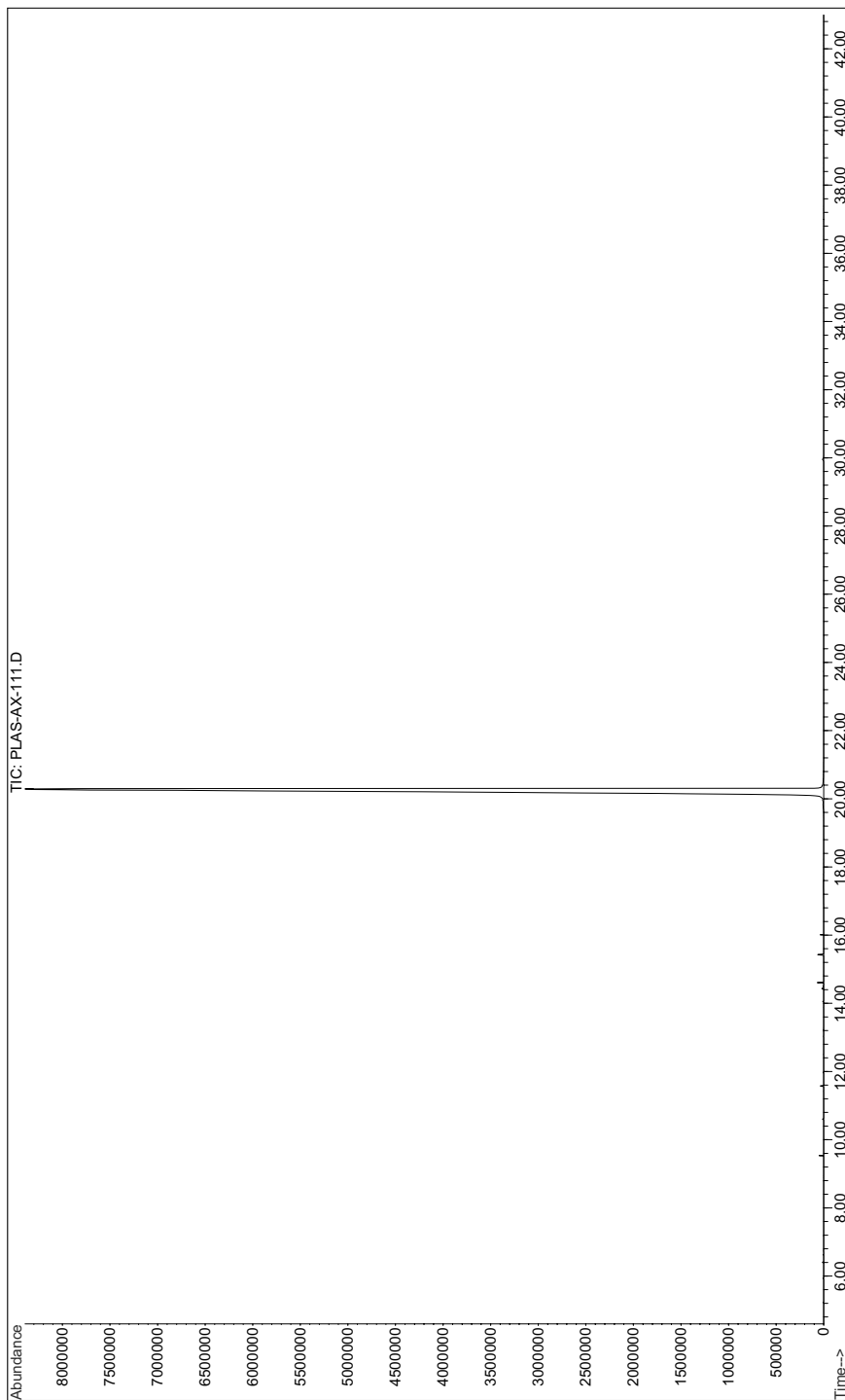
Analytical Information

Chromatogram for *Dibenzylhydroxylamine* - PLAS-AX-092

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



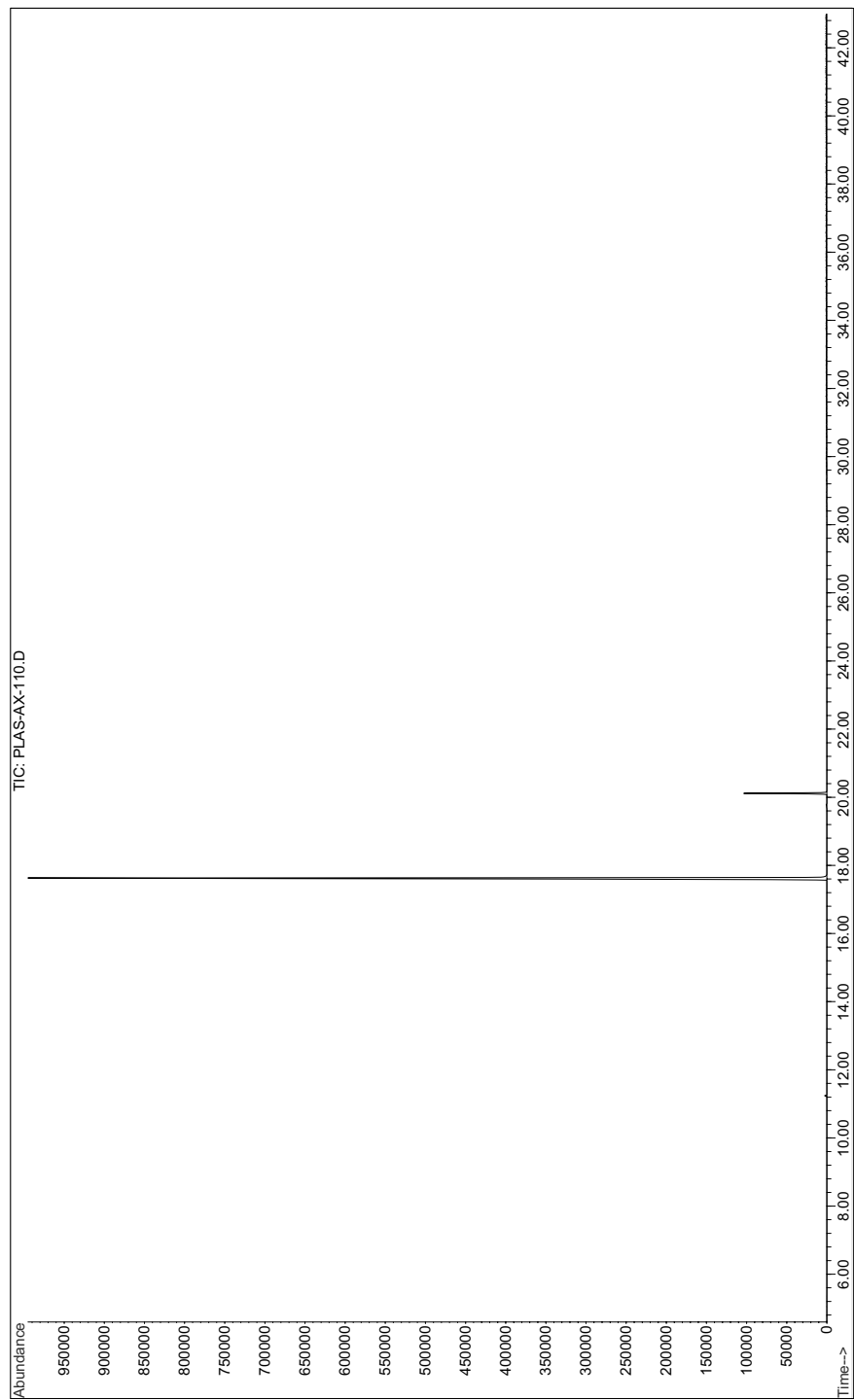
*Analytical Information***Chromatogram for *N,N'*-Dibutylthiourea - PLAS-AX-102****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for** 3,9-Bis(2,4-dicumylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane - PLAS-AX-111**Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for*Diethyl 3,5-Di-tert-butyl-4-hydroxybenzylphosphonate - PLAS-AX-110*

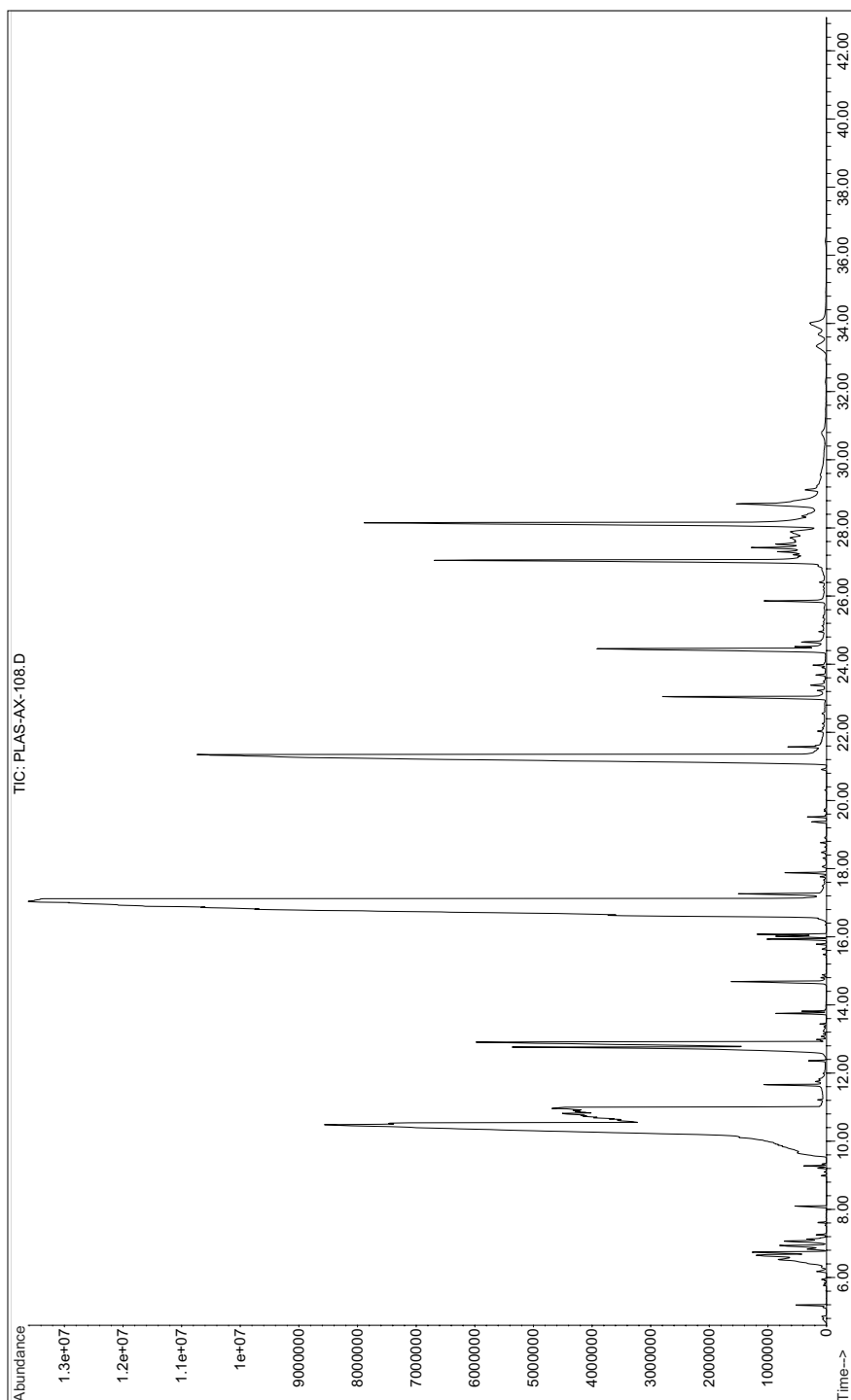
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *O,O'*-Diocetadecylpentaerythritol bis(phosphite) - PLAS-AX-108

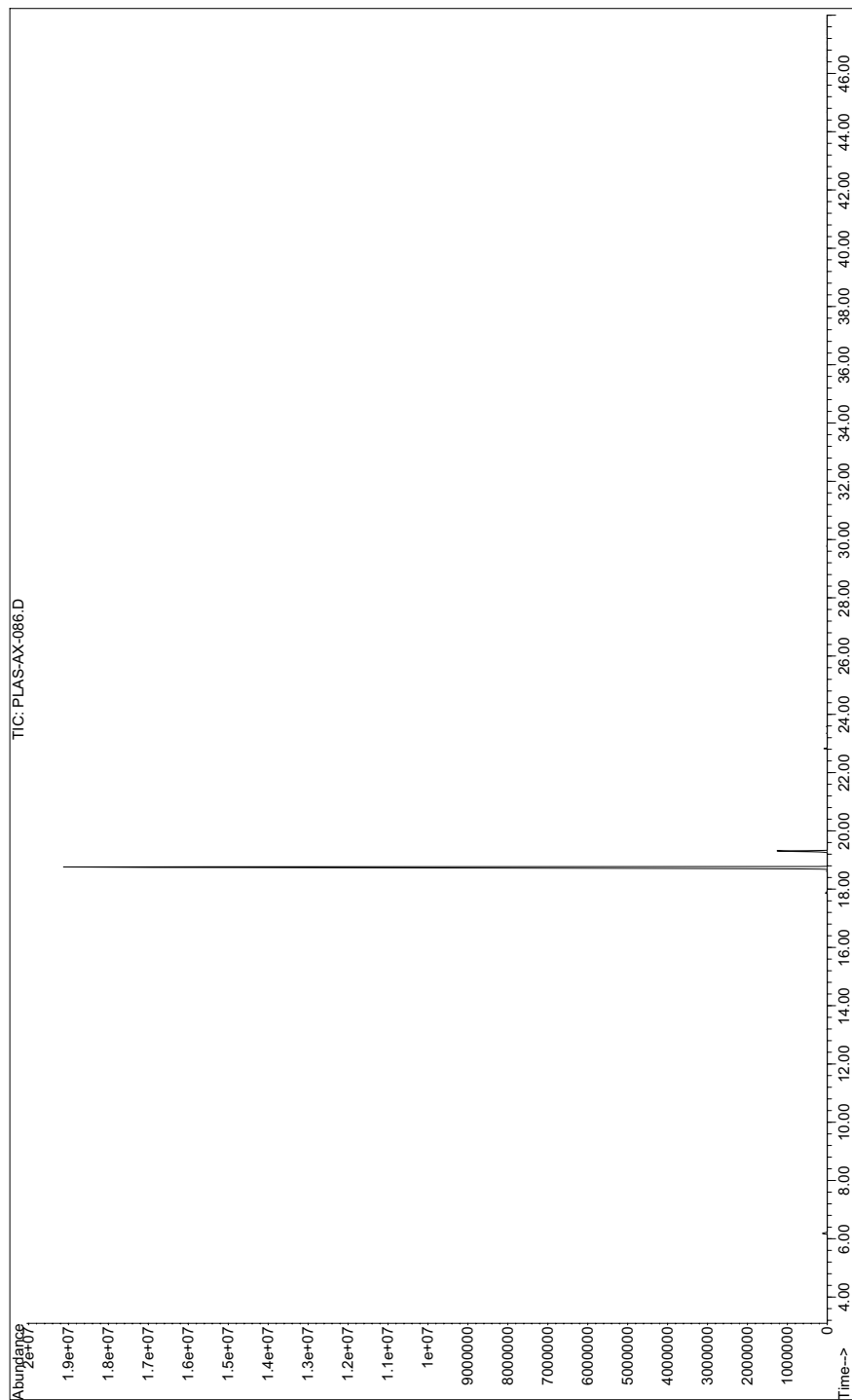
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Ethanox*[®] 310 - PLAS-AX-086

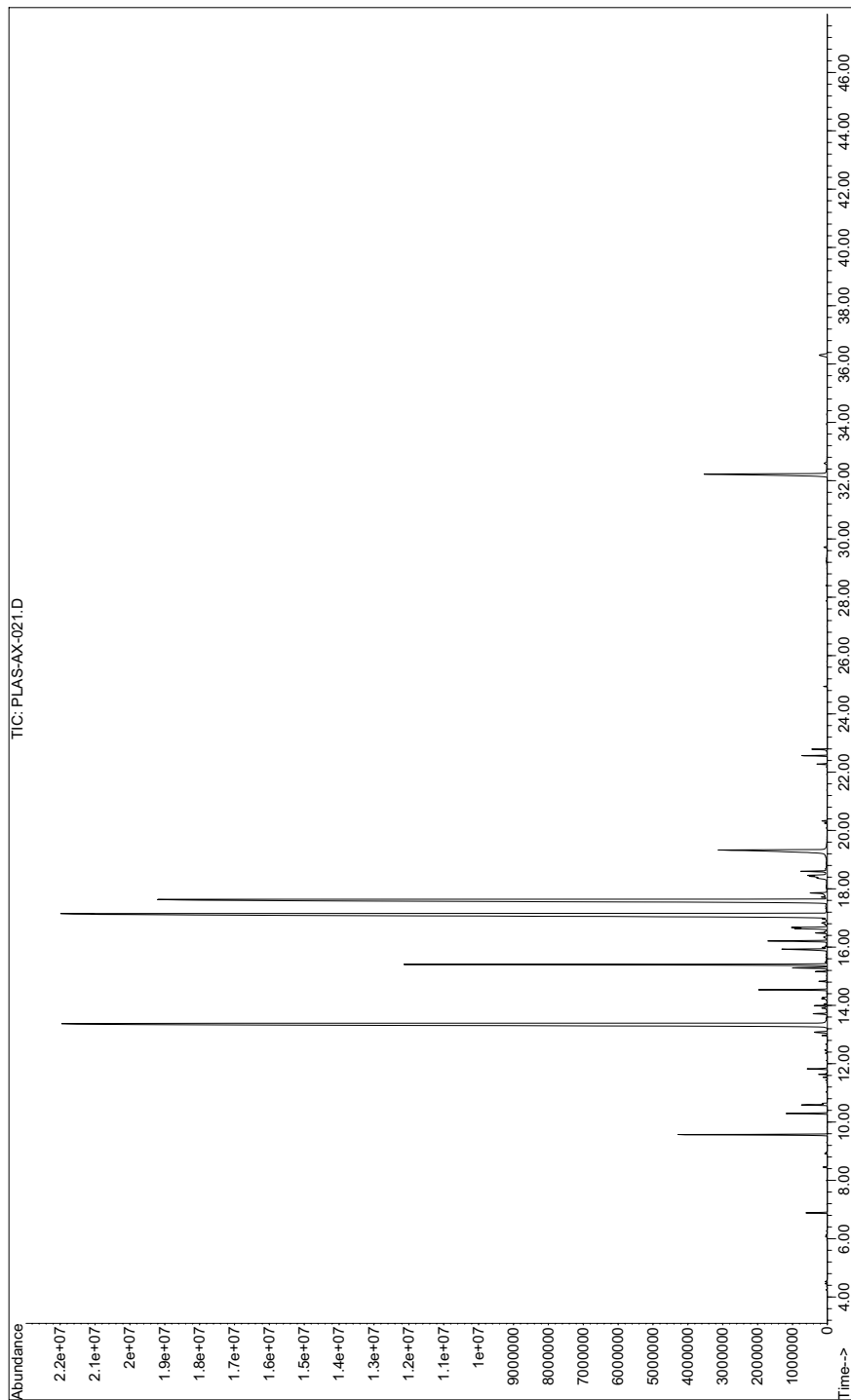
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

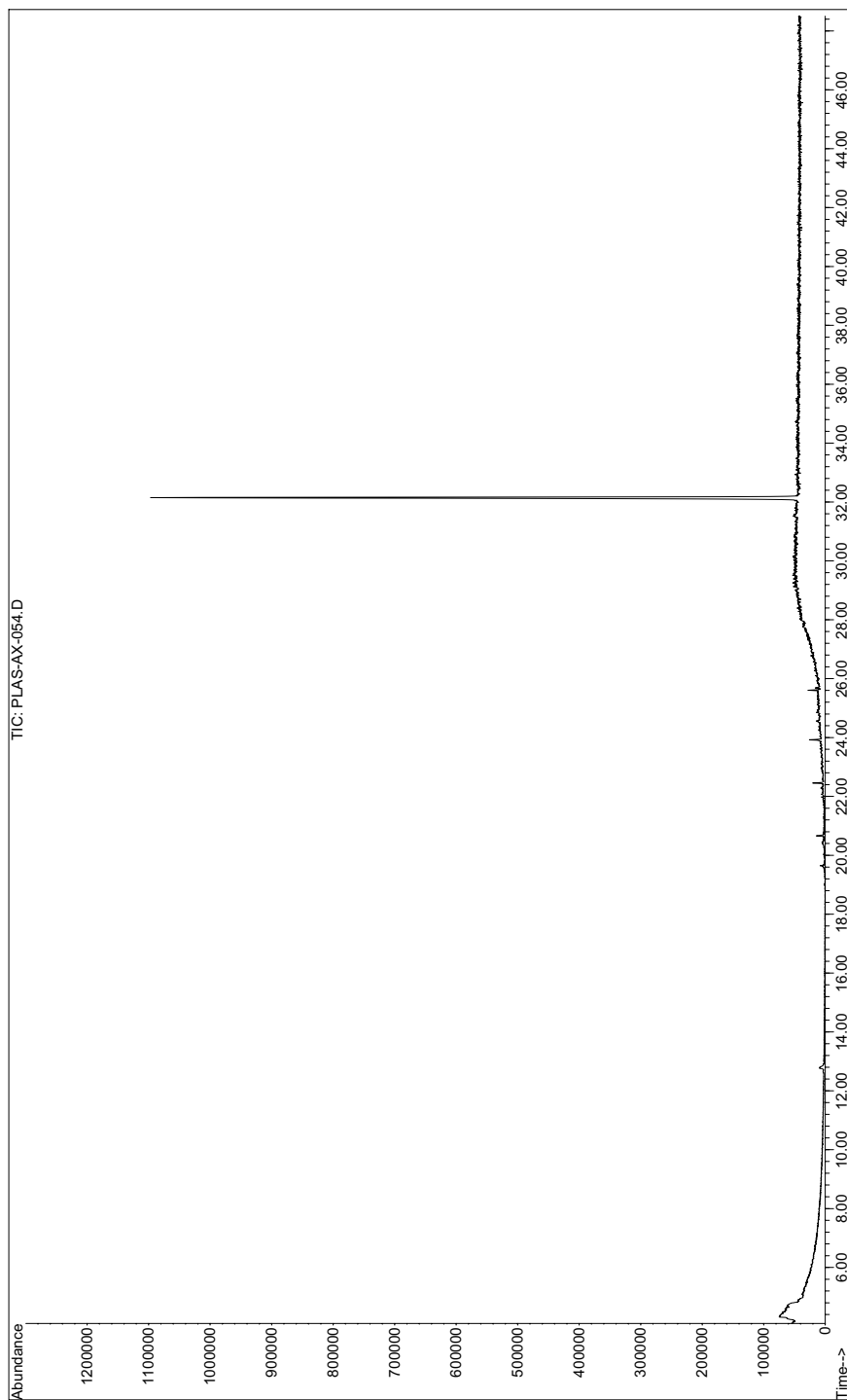


Analytical Information

Chromatogram for *Ethanox*[®] 330 - PLAS-AX-021

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



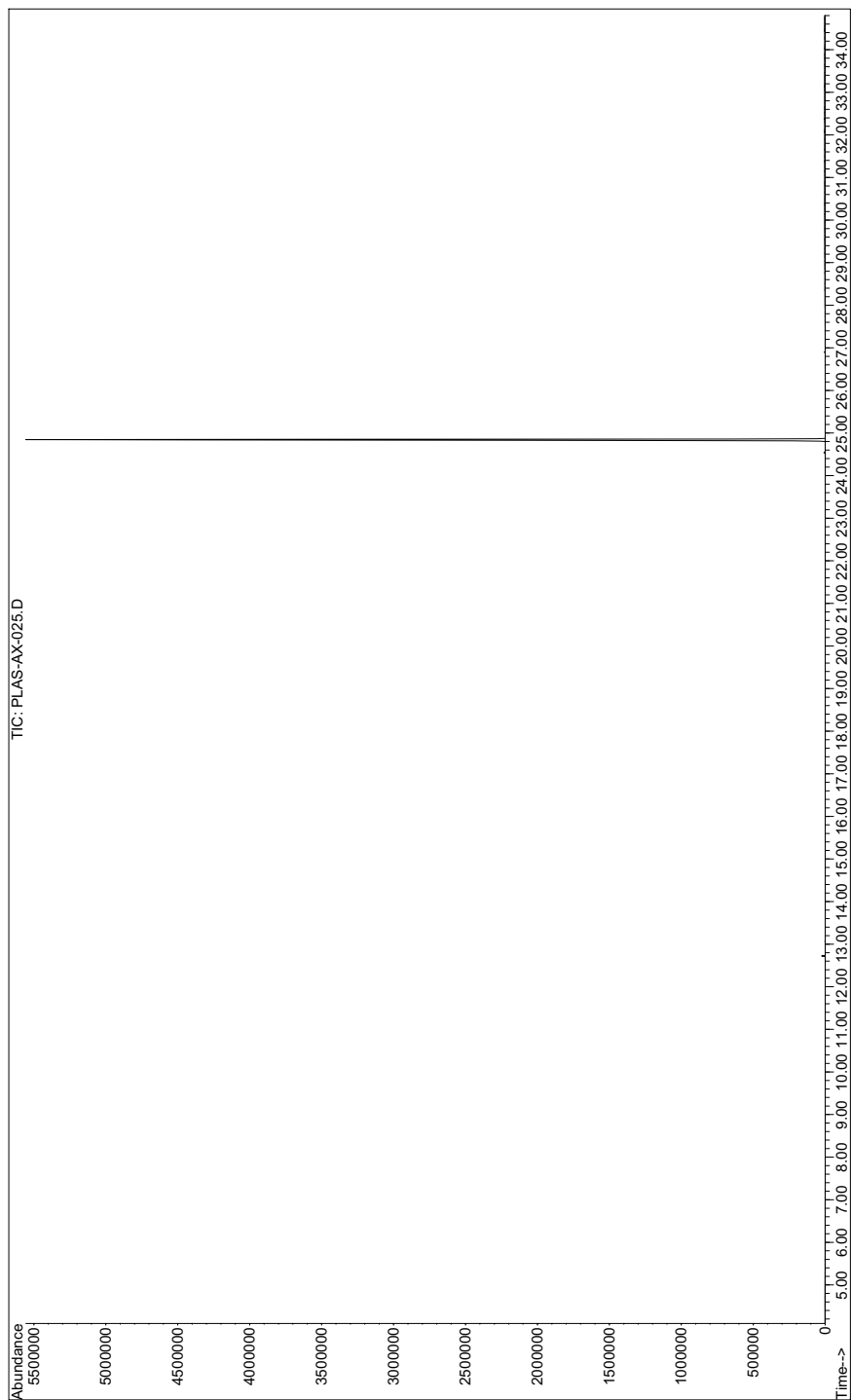
*Analytical Information***Chromatogram for *Ethanox*[®] 376 - PLAS-AX-054****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *Ethanol*[®] 702 - PLAS-AX-025

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

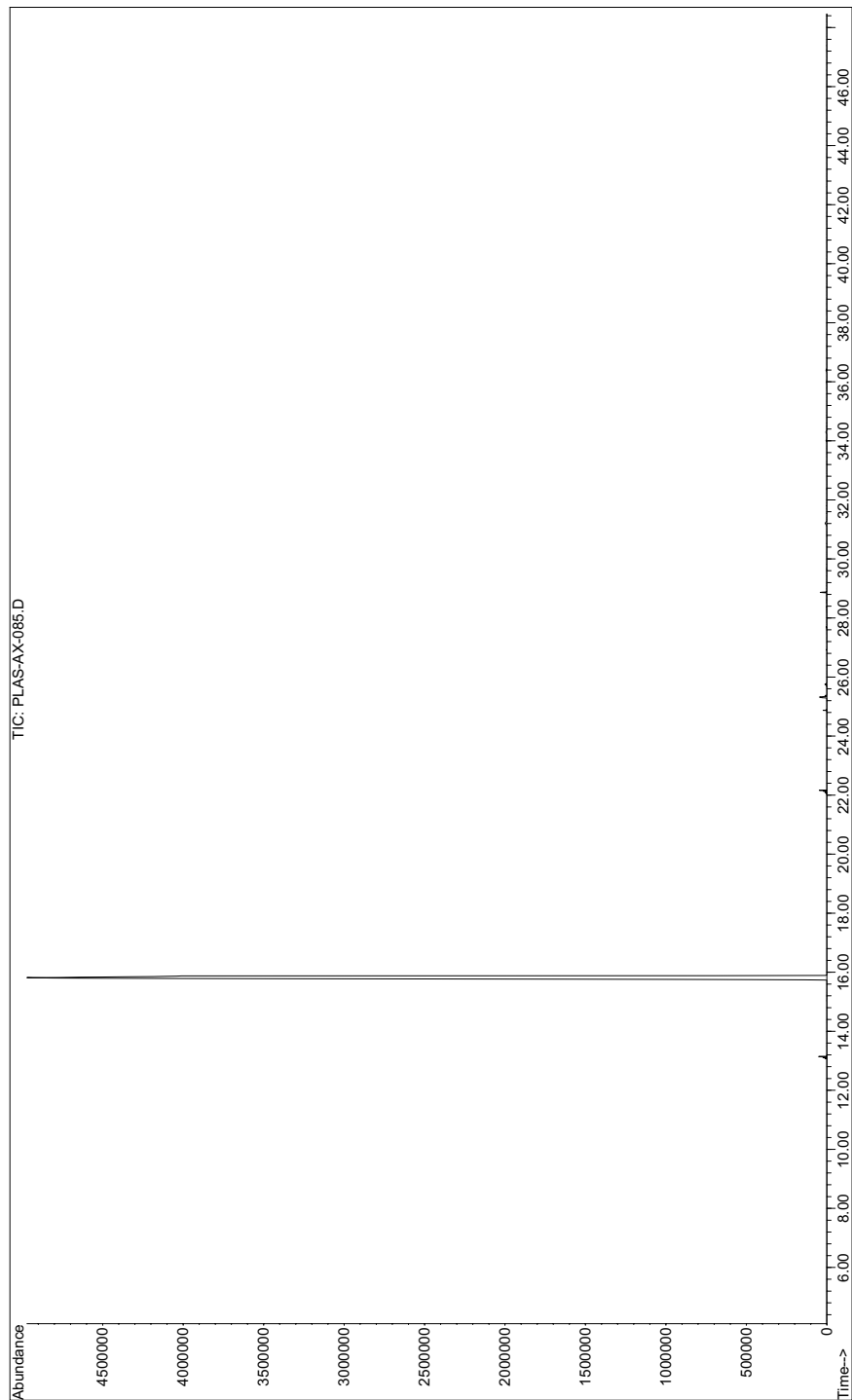
Inj Temp=250 °C, Det=MSD

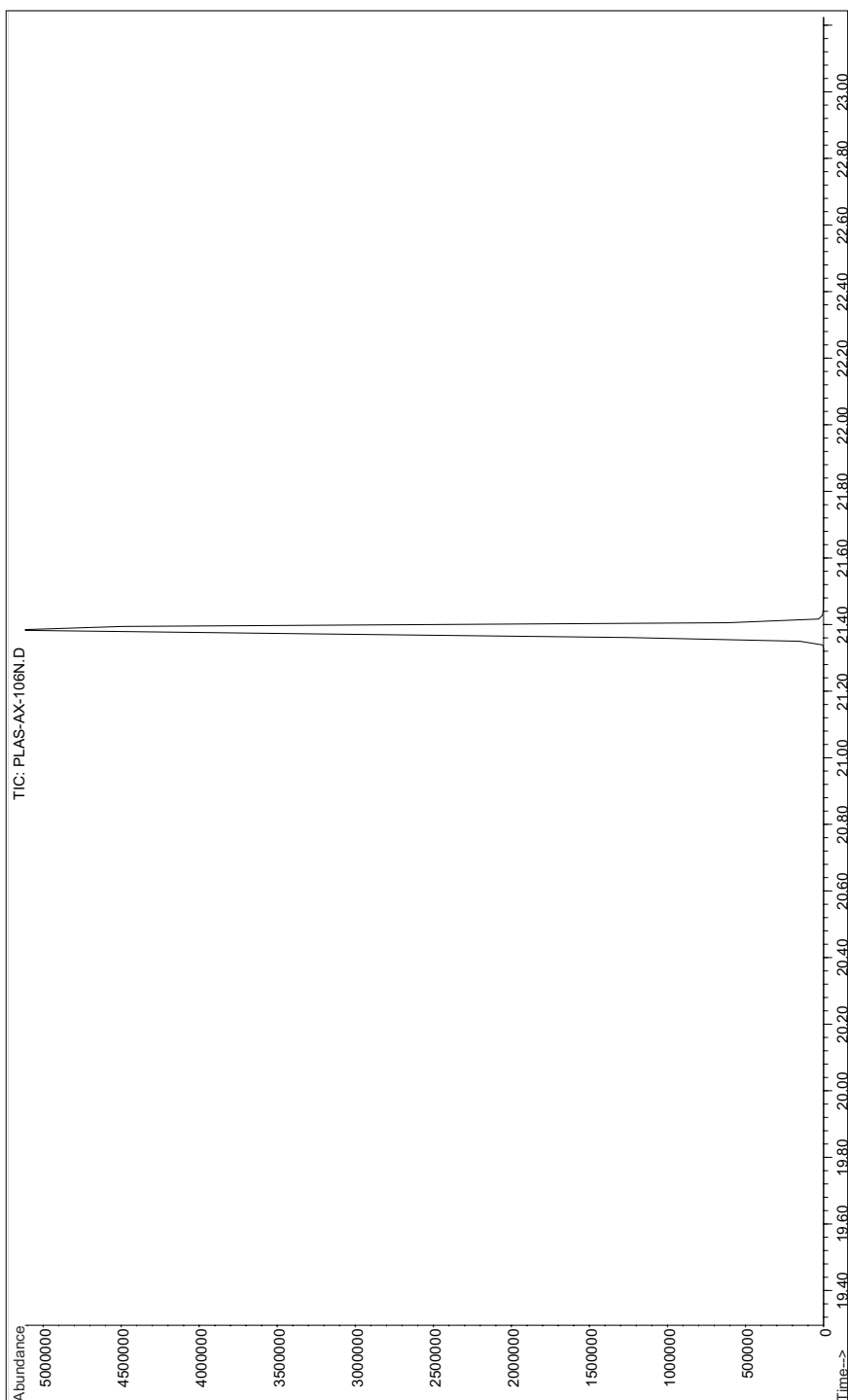


Analytical Information

Chromatogram for *Ethanox*[®] 703 - PLAS-AX-085

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

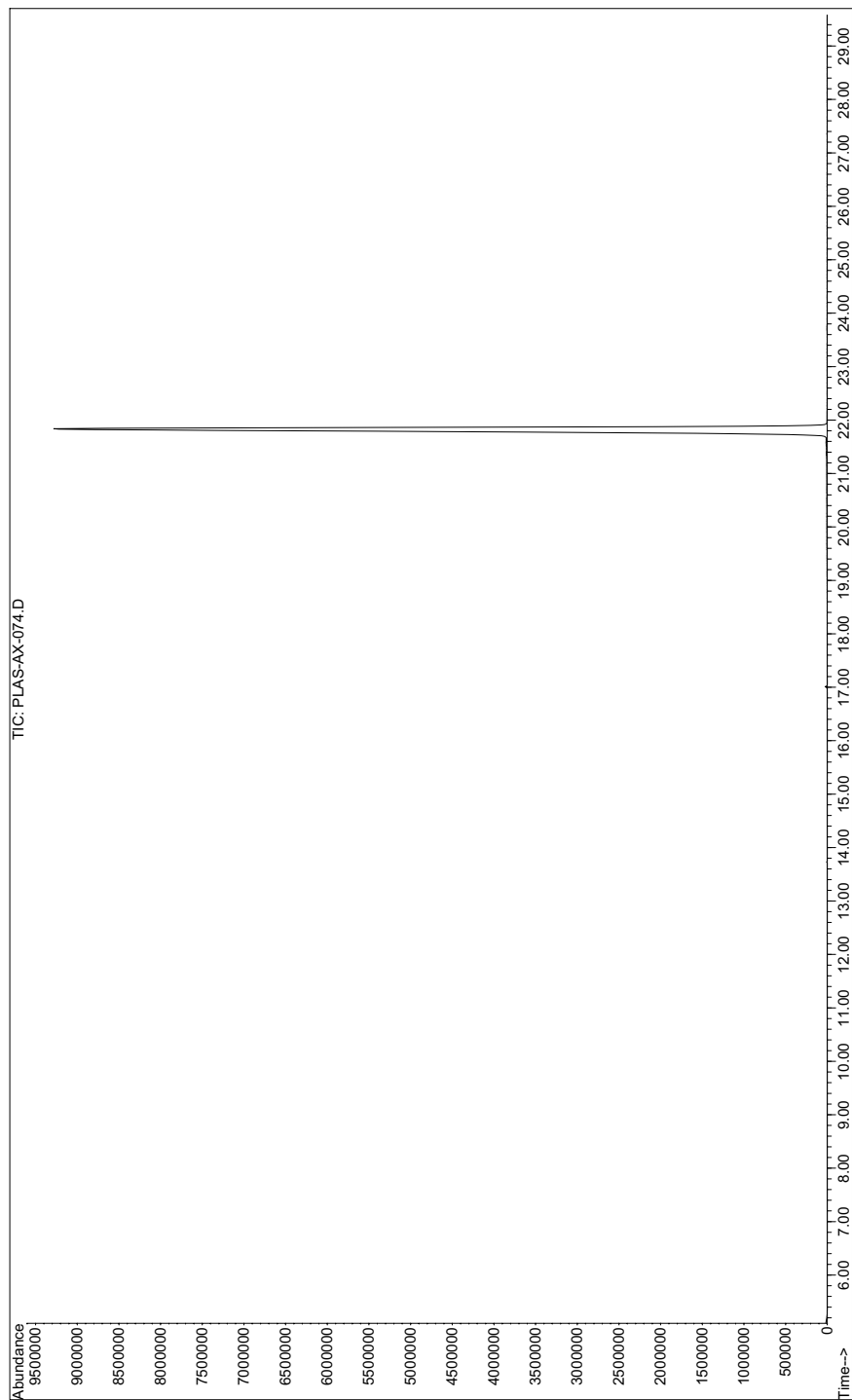


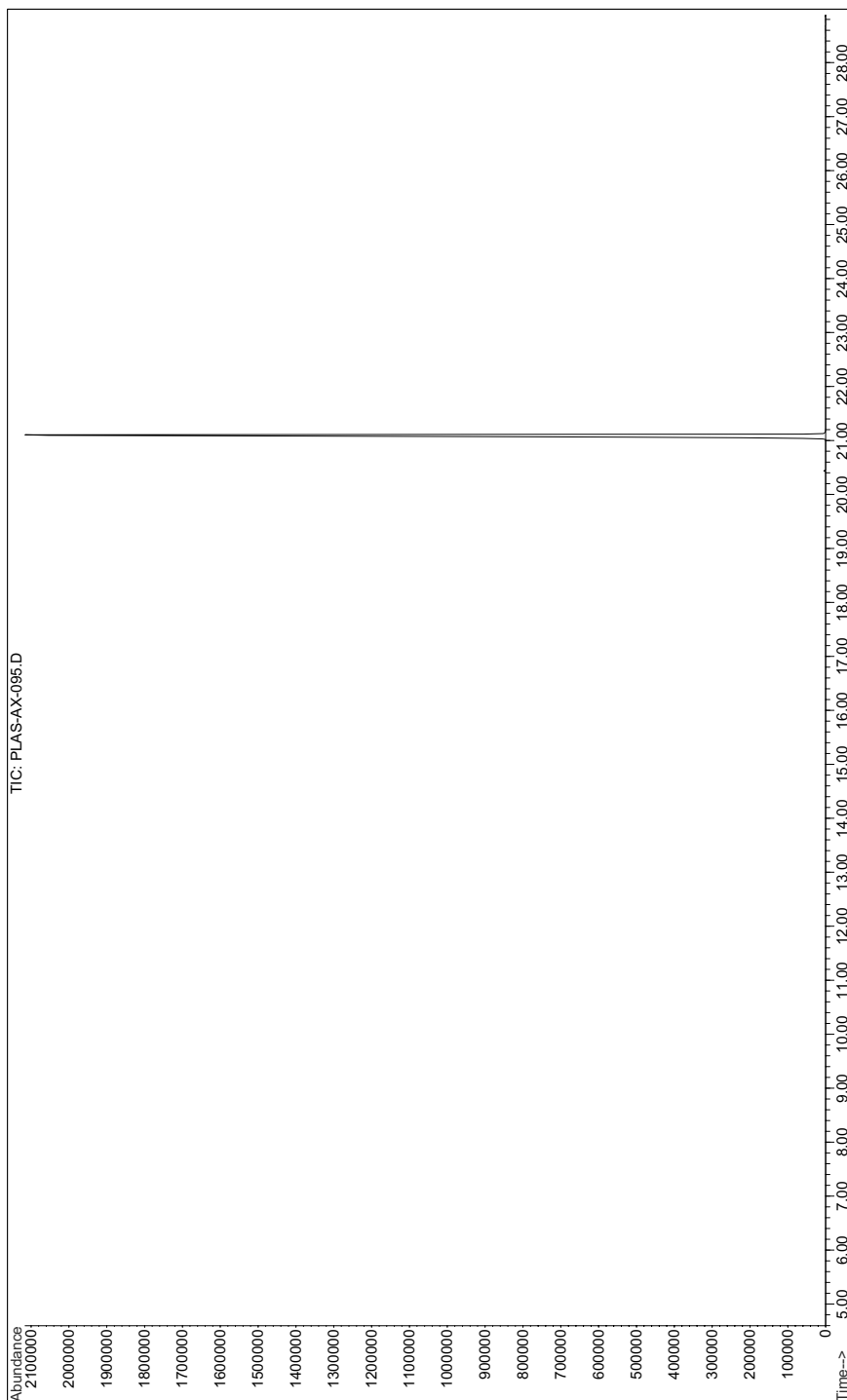
*Analytical Information***Chromatogram for 2,2'-Ethylidene-bis(4,6-di-tert-butylphenol) - PLAS-AX-106****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

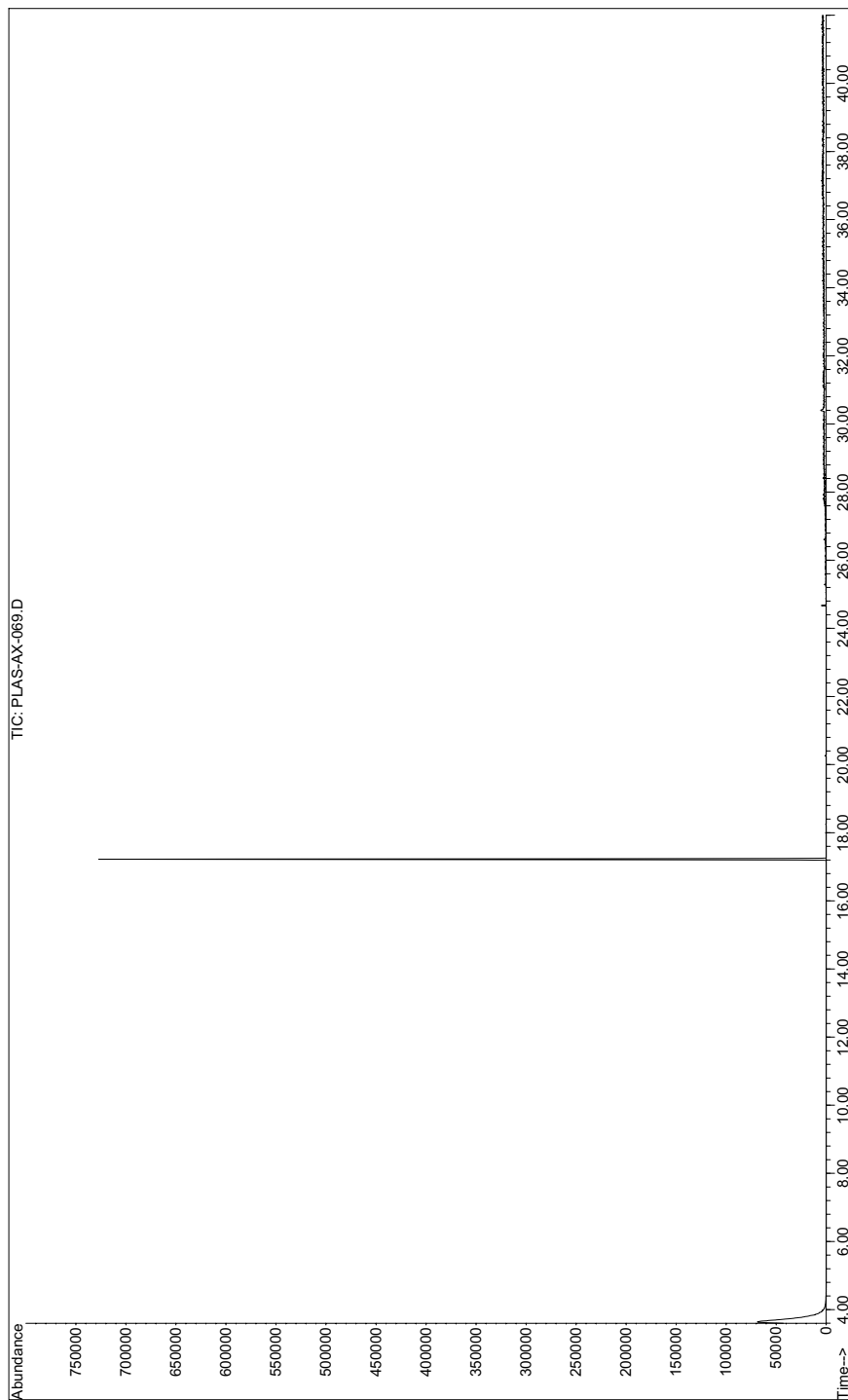
Analytical Information

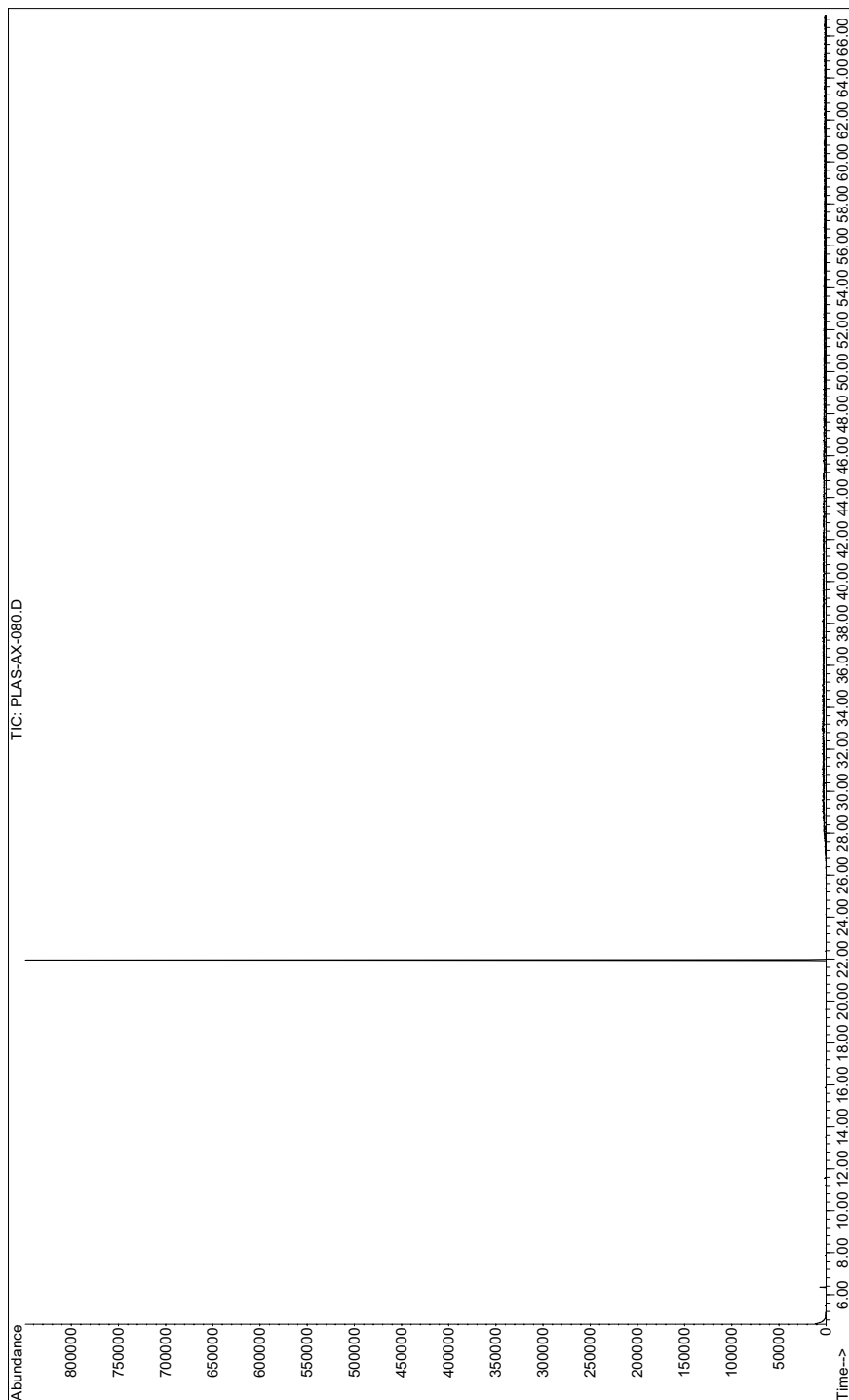
Chromatogram for*Ethaphos*[®] 368 - *PLAS-AX-074*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



*Analytical Information***Chromatogram for 2-(2'-Hydroxy-3',5'-di-tert-amylphenyl) benzotriazole - PLAS-AX-095****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

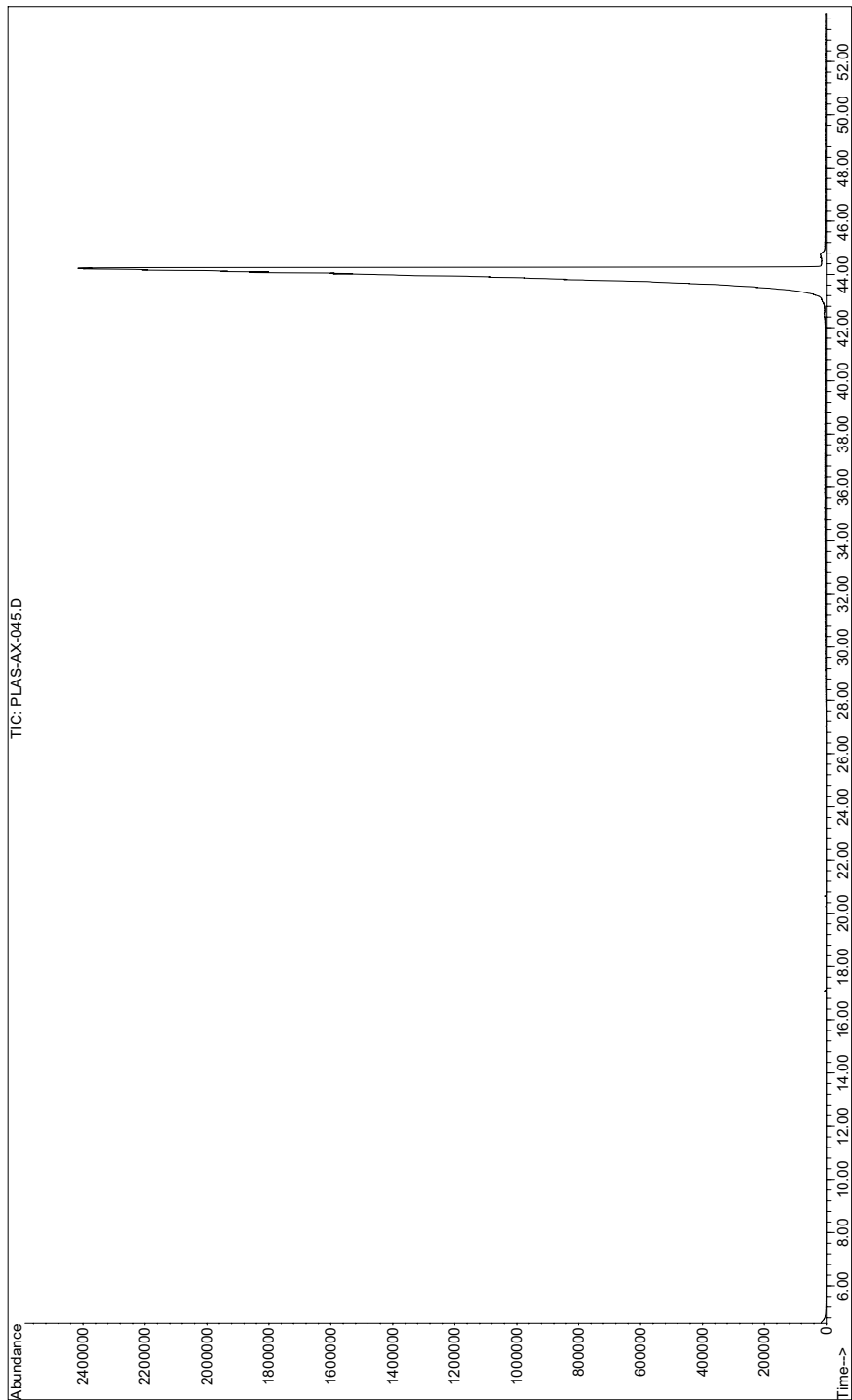
*Analytical Information***Chromatogram for Irganox[®] 1035 - PLAS-AX-069****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

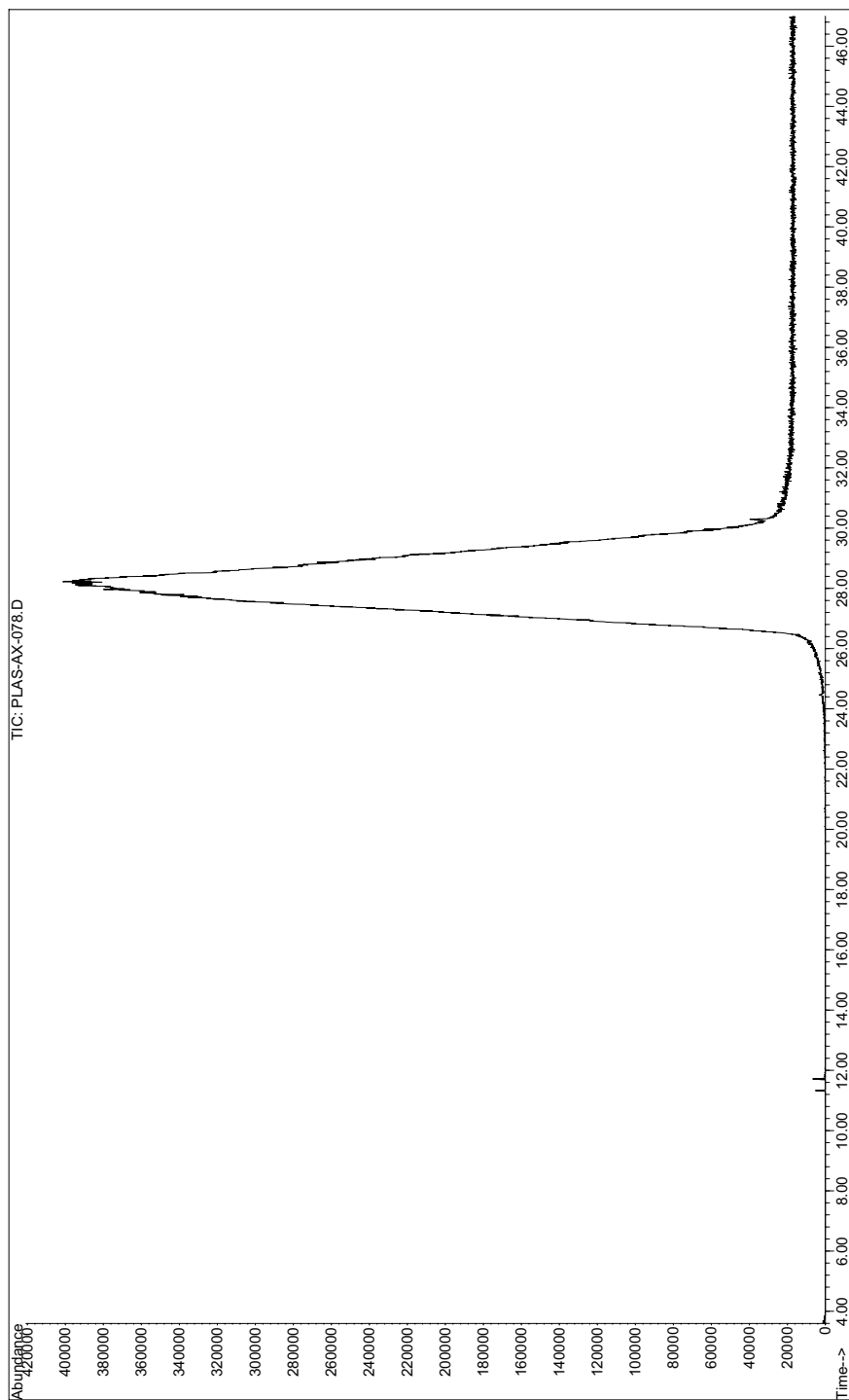
*Analytical Information***Chromatogram for Irganox[®] 1081 - PLAS-AX-080****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

Analytical Information

Chromatogram for Irganox® 259 - PLAS-AX-045

Analytical Conditions Summary 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD

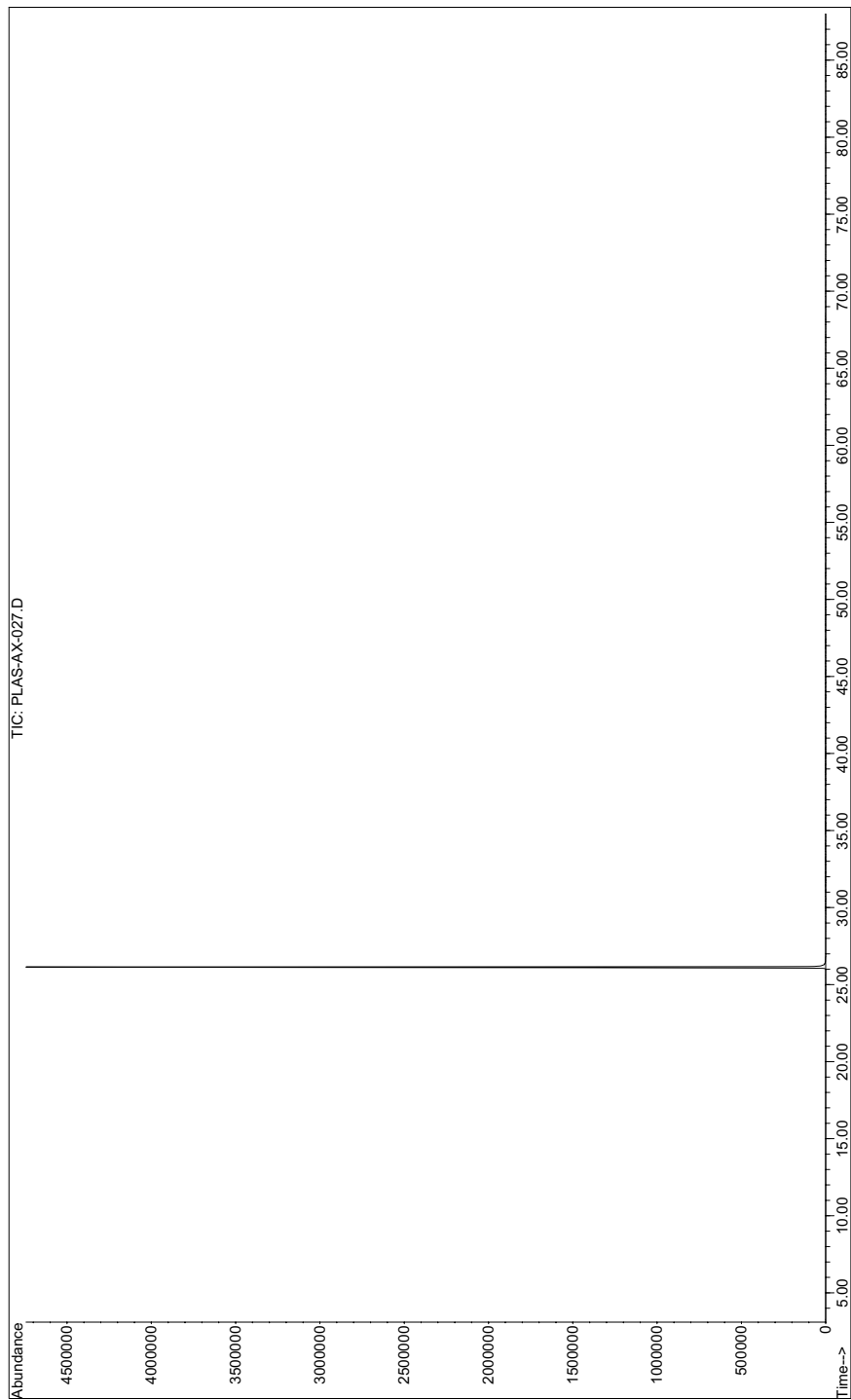


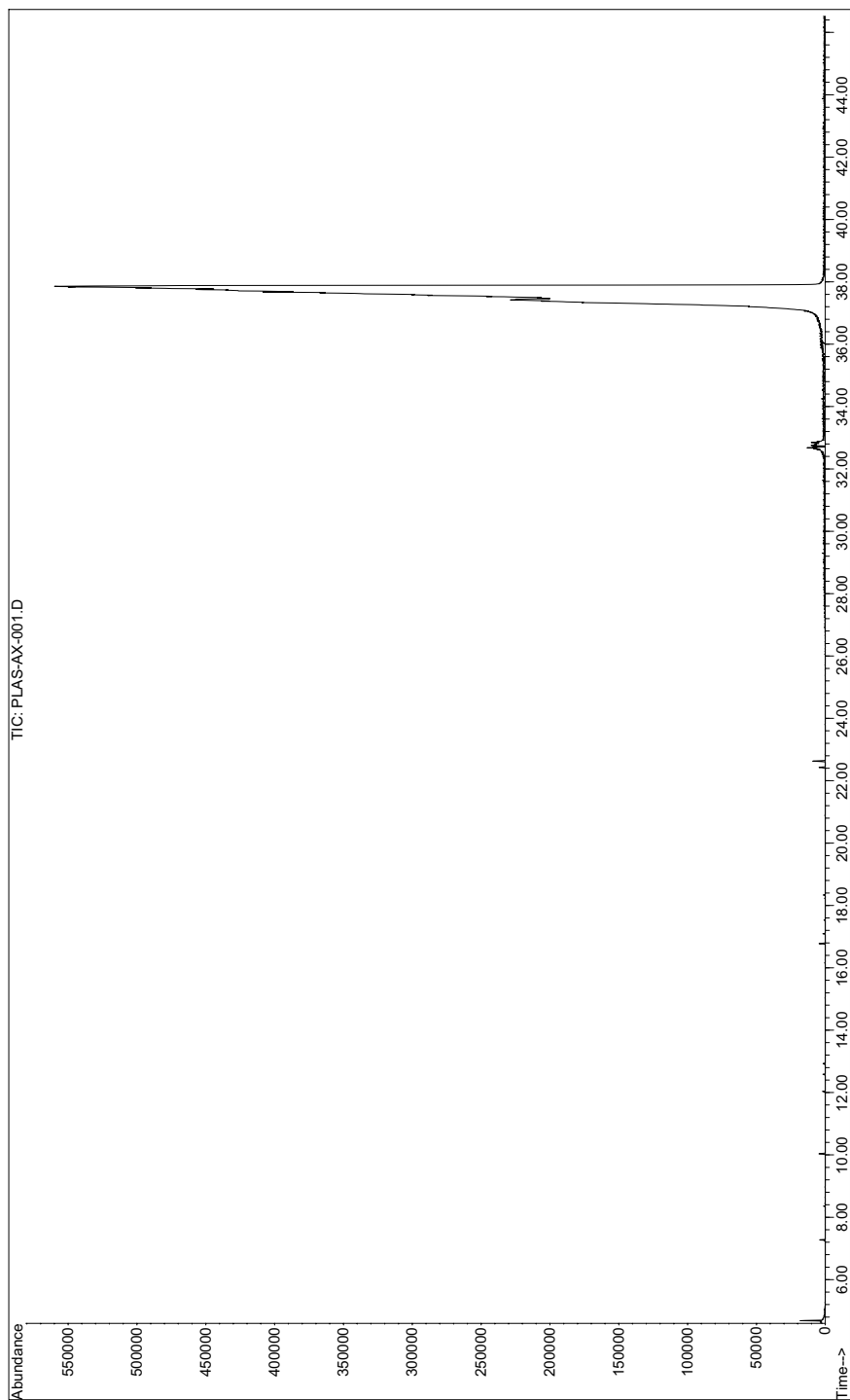
*Analytical Information***Chromatogram for Irganox® 3114 FF - PLAS-AX-078****Analytical Conditions Summary** 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD

Analytical Information

Chromatogram for Irganox® E 201 - PLAS-AX-027

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

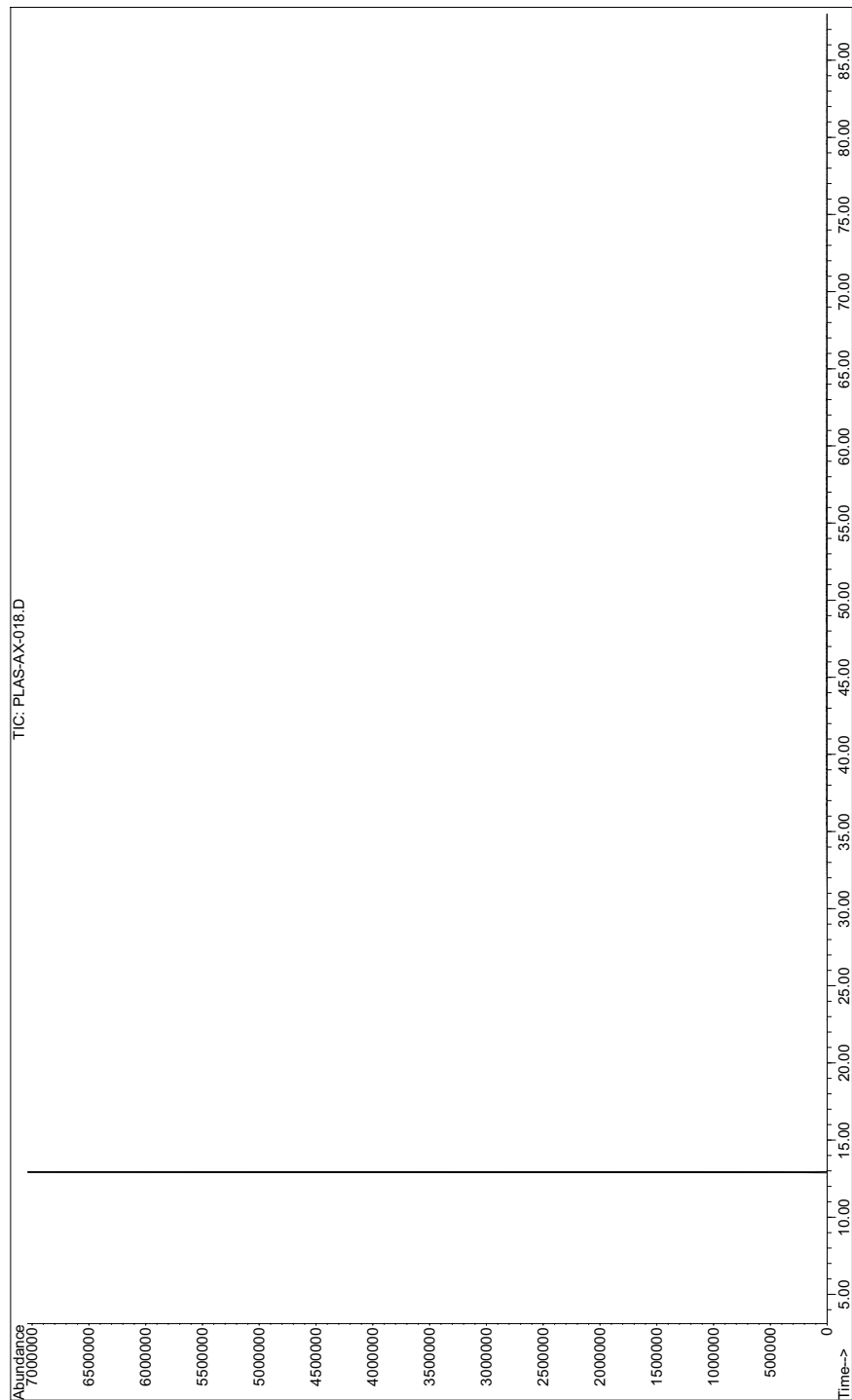


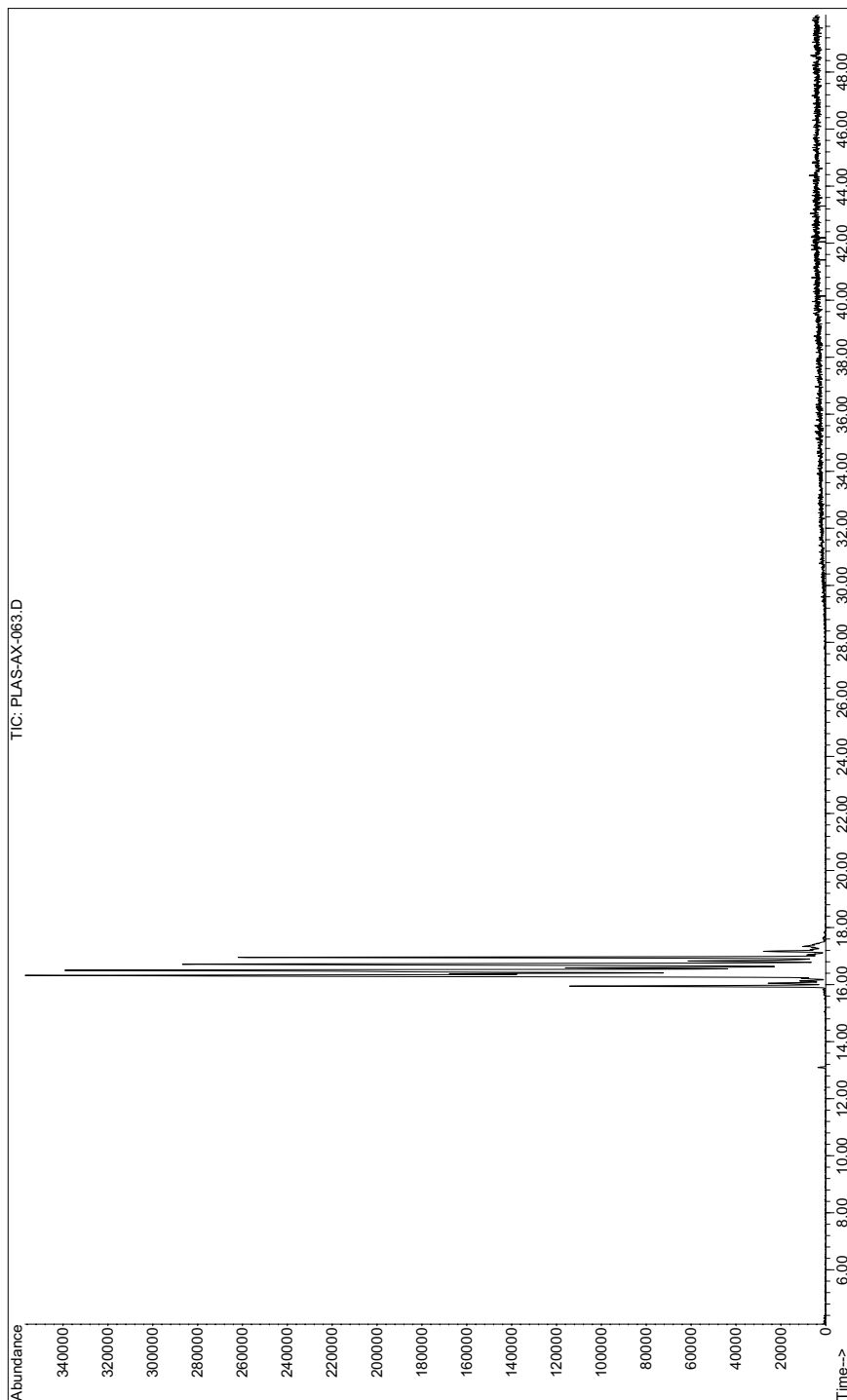
*Analytical Information***Chromatogram for Irganox[®] MD 1024 - PLAS-AX-001****Analytical Conditions Summary** 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD

Analytical Information

Chromatogram for Isonox[®] 132 - PLAS-AX-018

Analytical Conditions Summary 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD

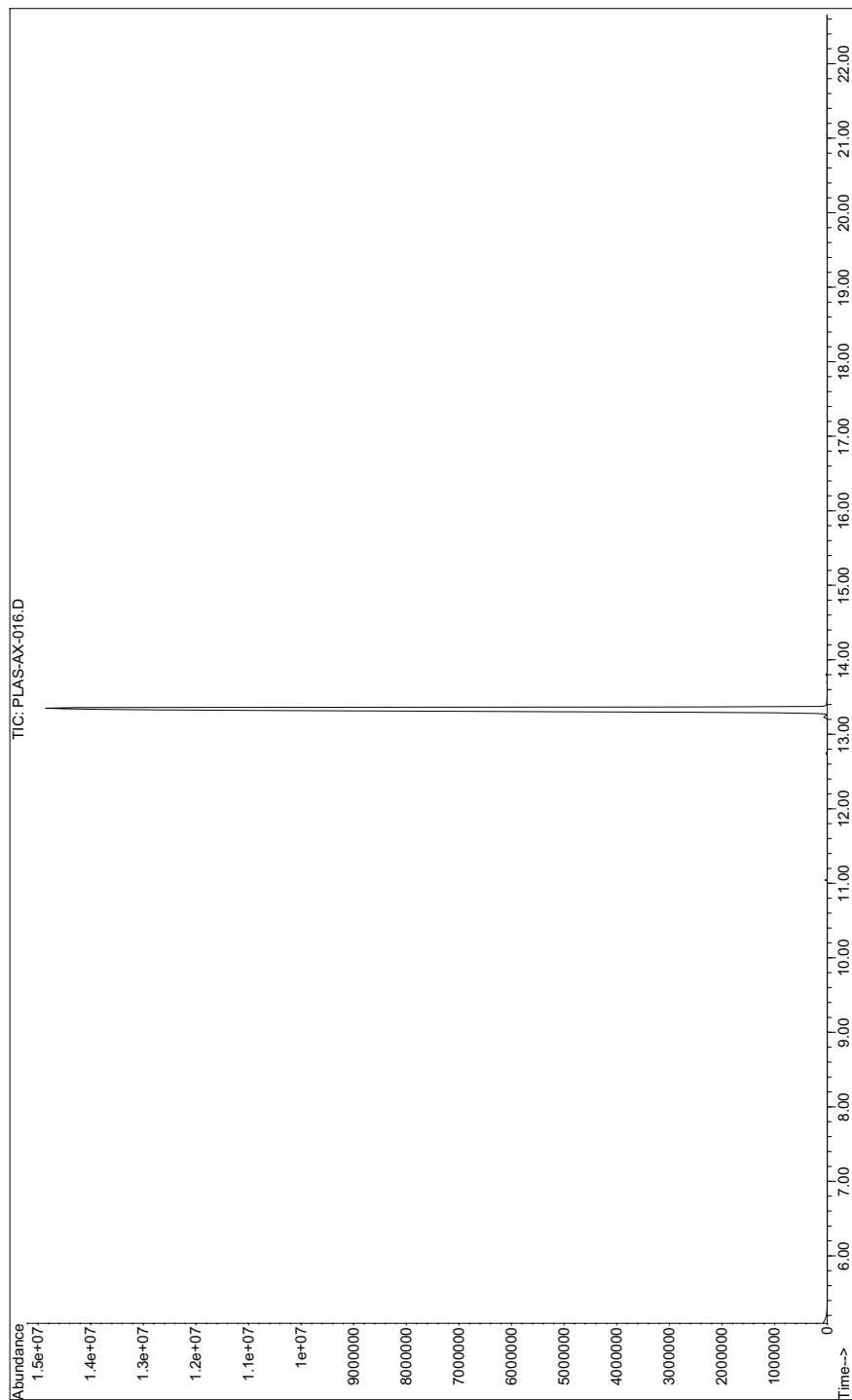


*Analytical Information***Chromatogram for *Isonox*[®] 232 - PLAS-AX-063****Analytical Conditions Summary** 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD

Analytical Information

Chromatogram for *Lowinox® AH25 - PLAS-AX-016*

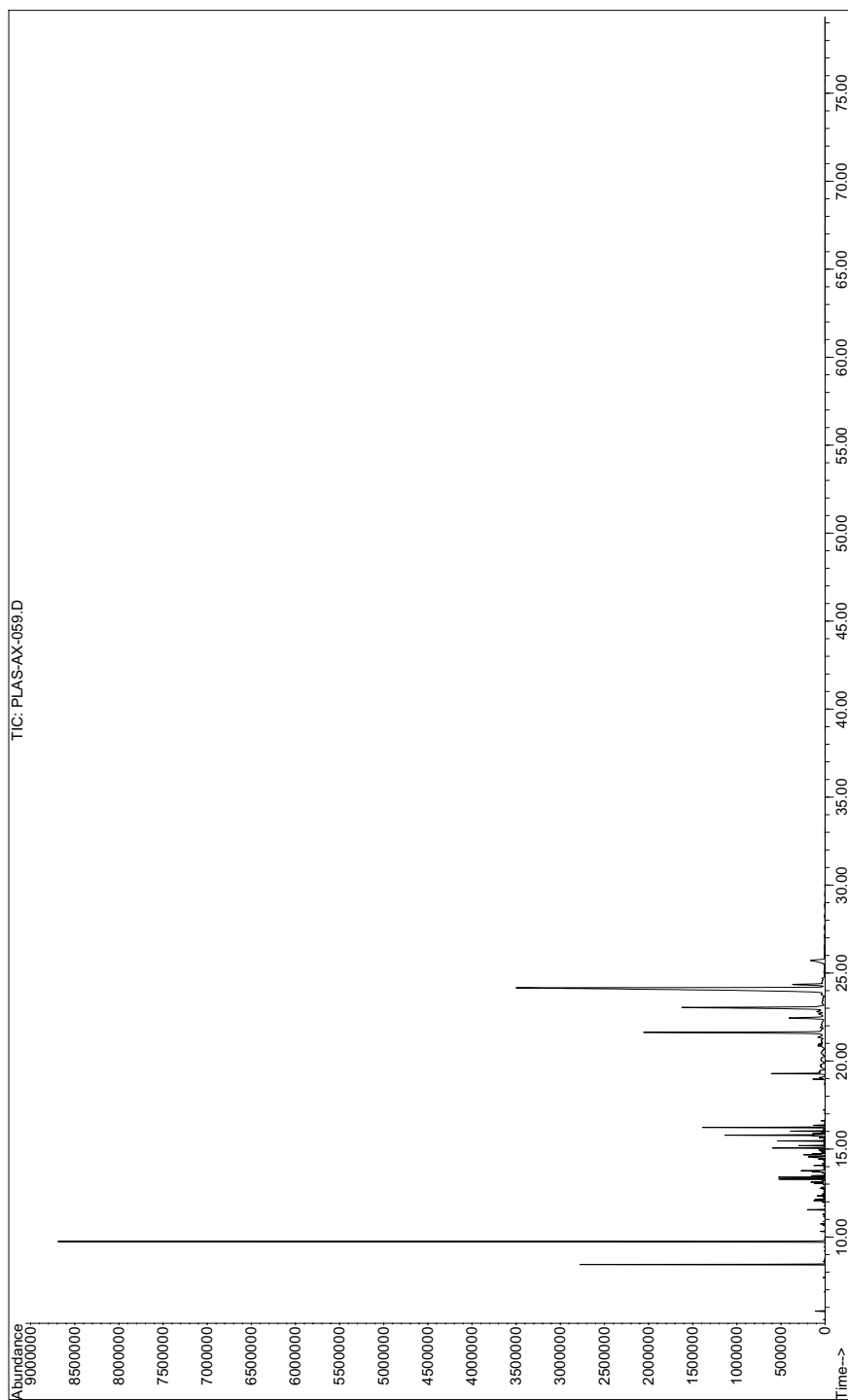
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for*Lowinox® CPL - PLAS-AX-059*

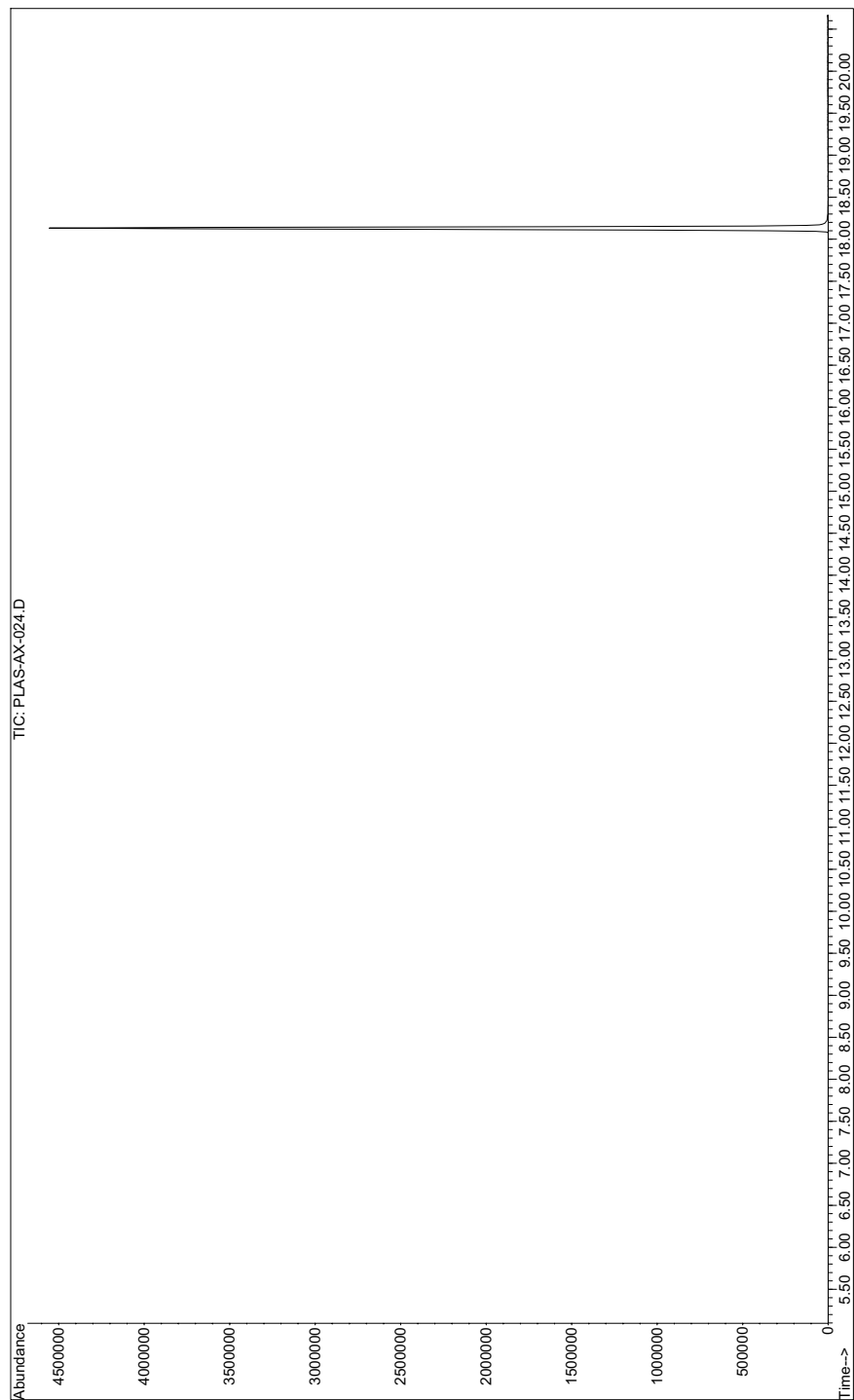
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

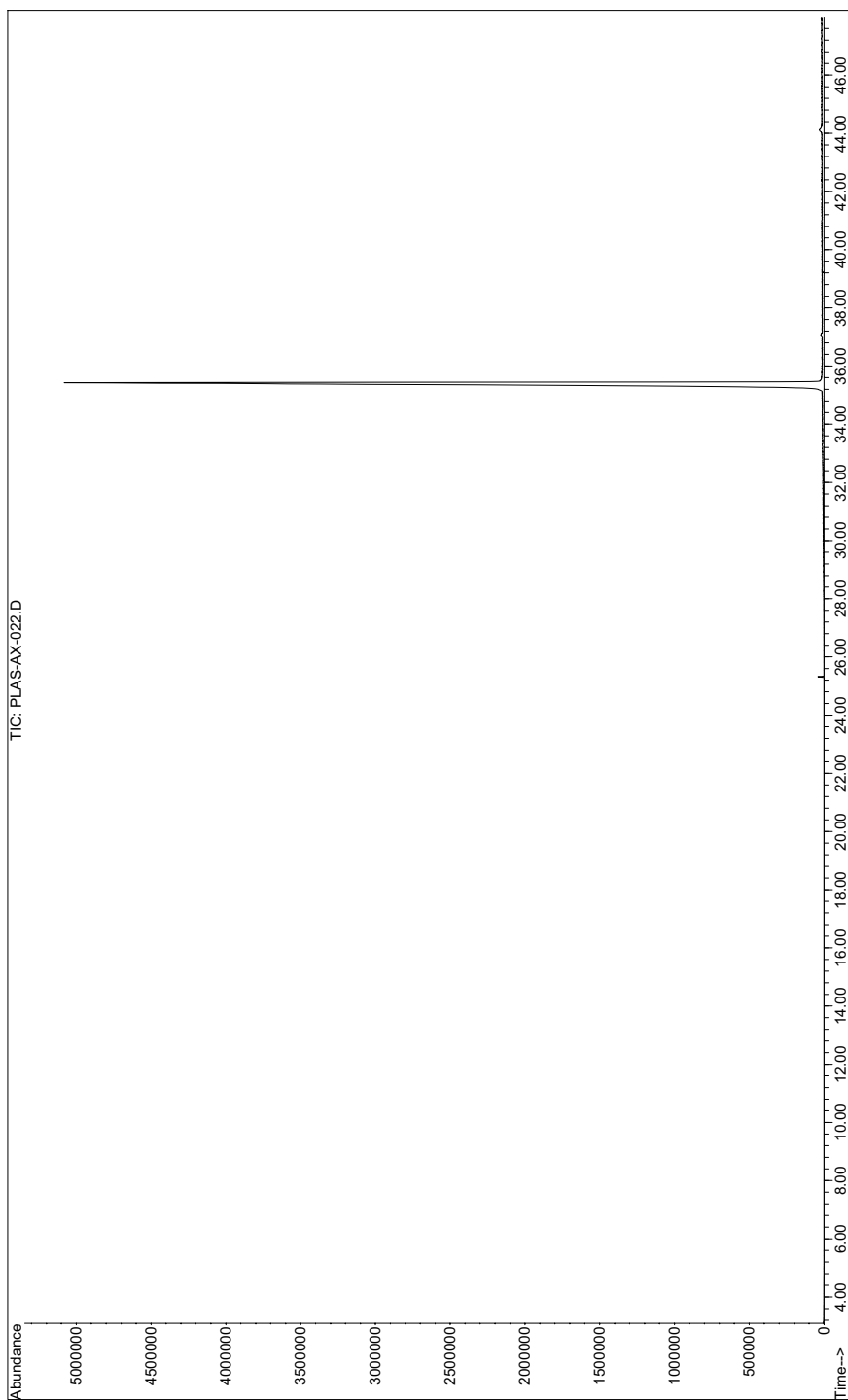


Analytical Information

Chromatogram for *Lowinox® TBM-6 - PLAS-AX-024*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

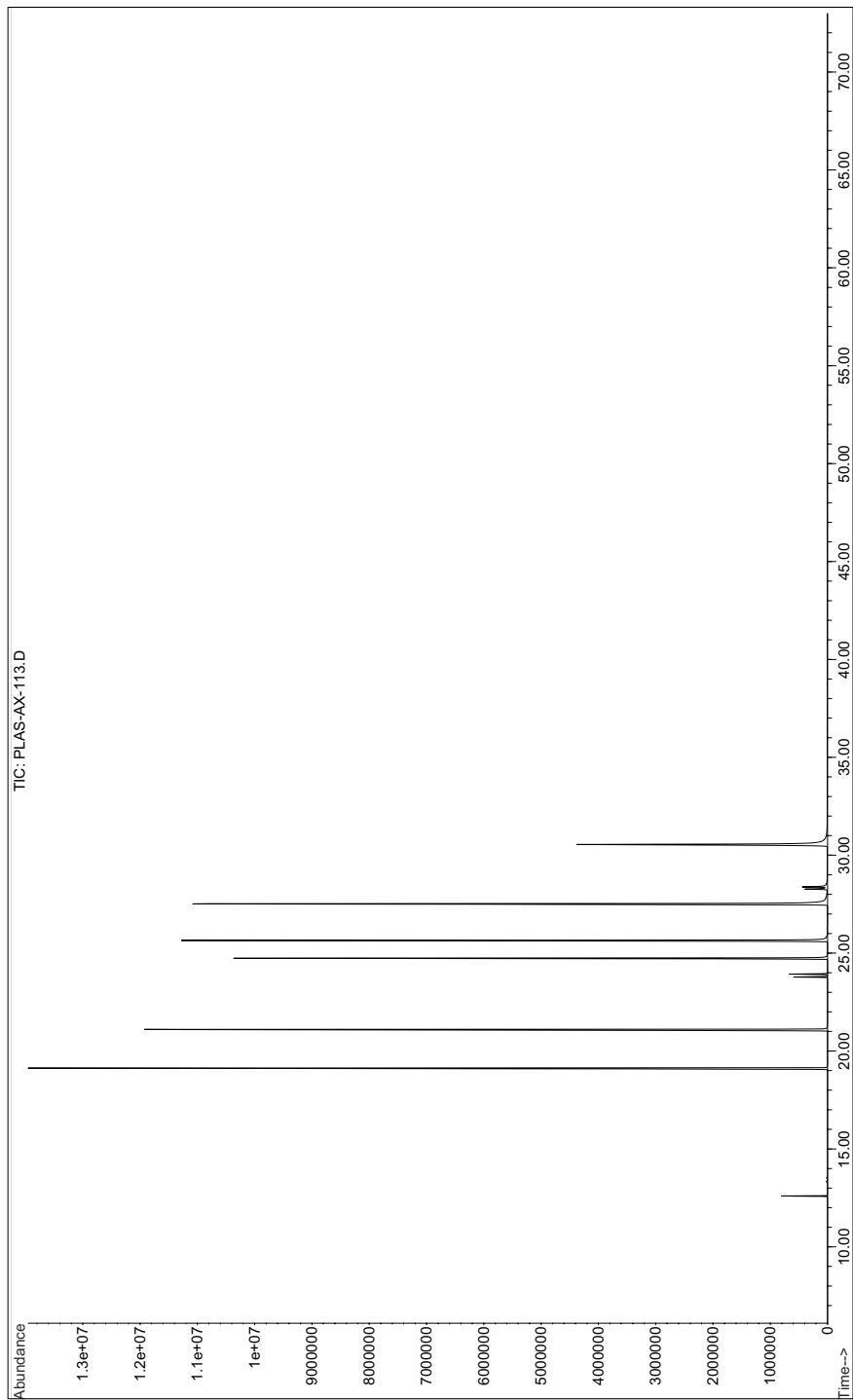


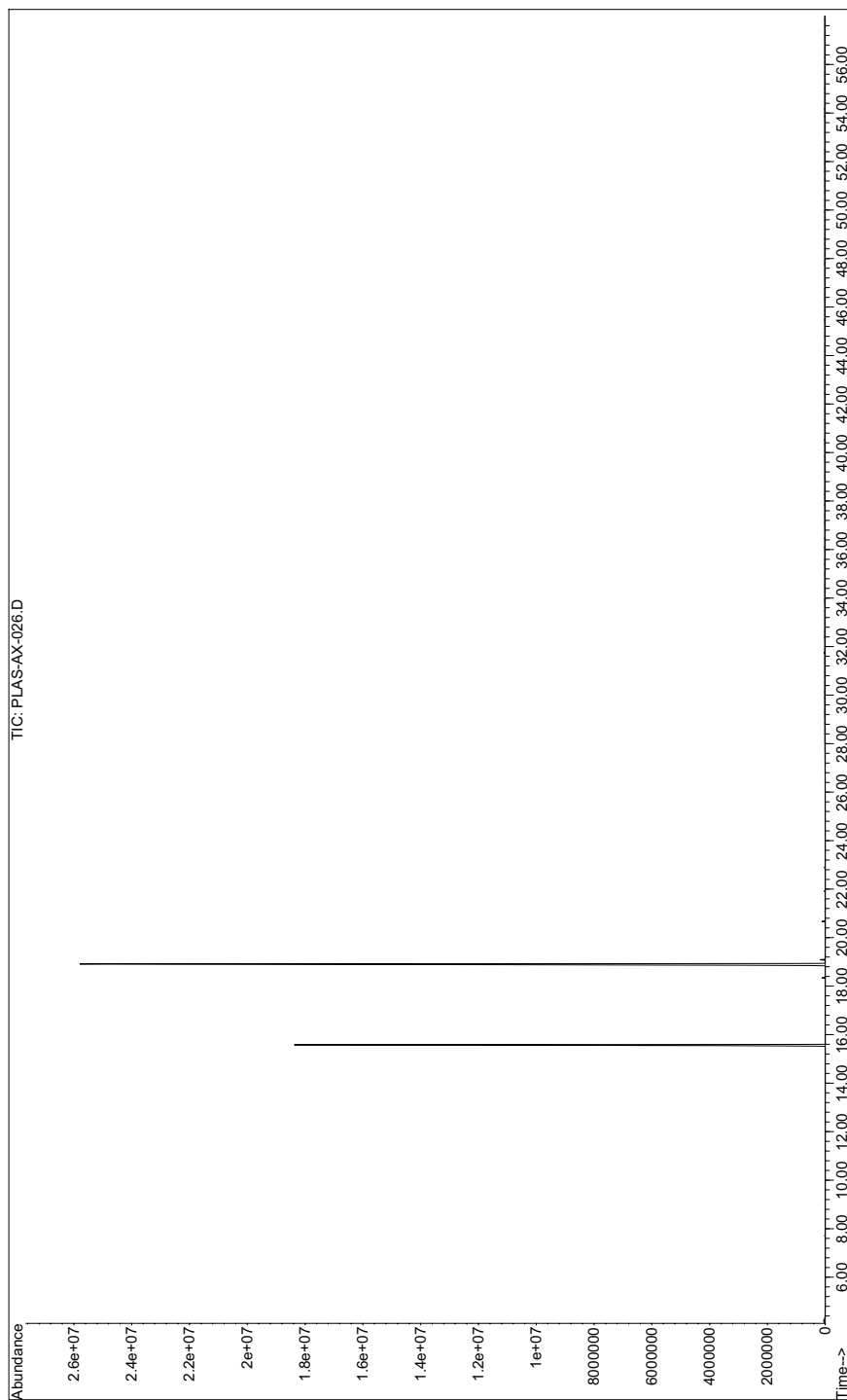
*Analytical Information***Chromatogram for Naugard[®] 445 - PLAS-AX-022****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

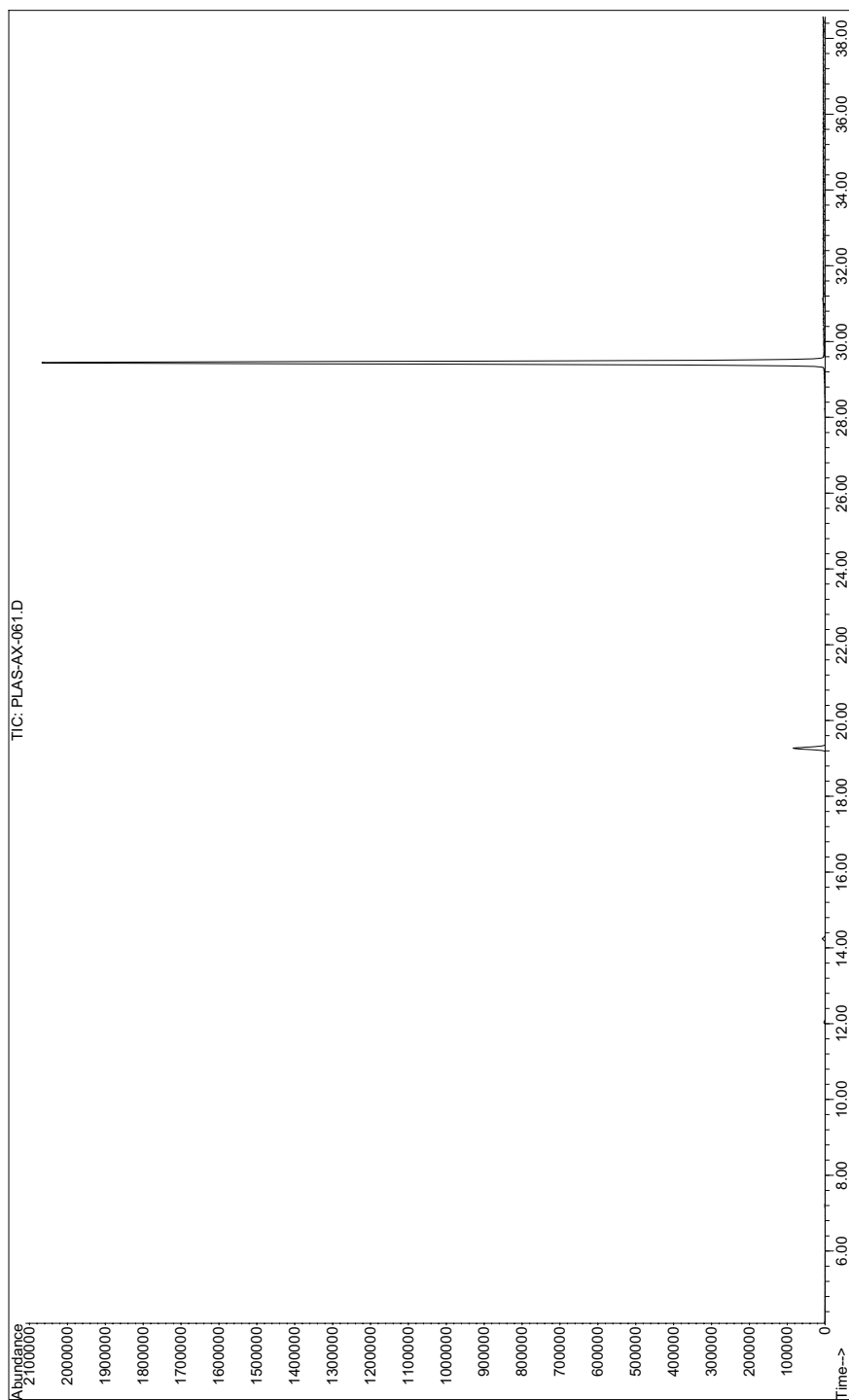
Analytical Information

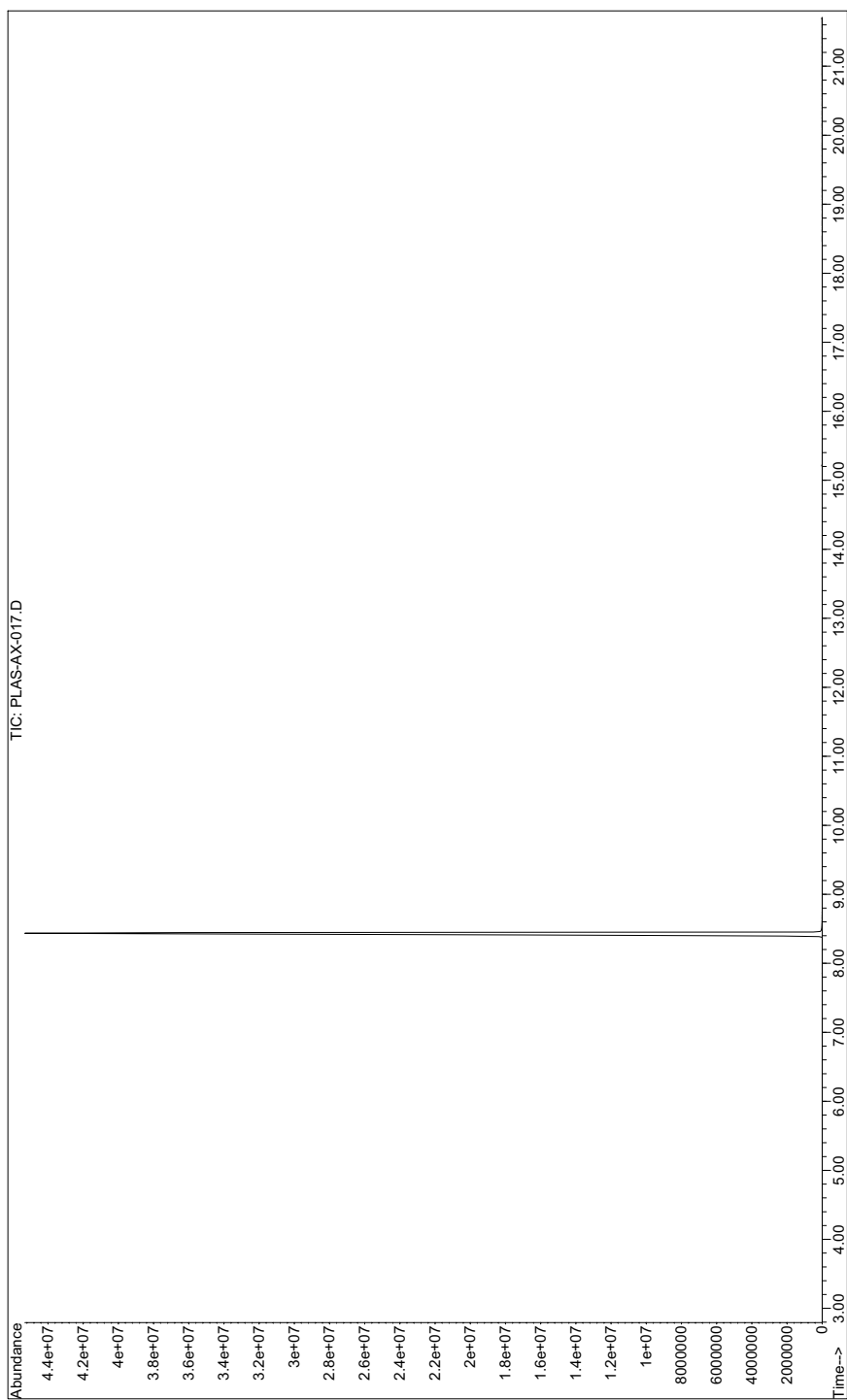
Chromatogram for*Naugard 635 - PLAS-AX-113*

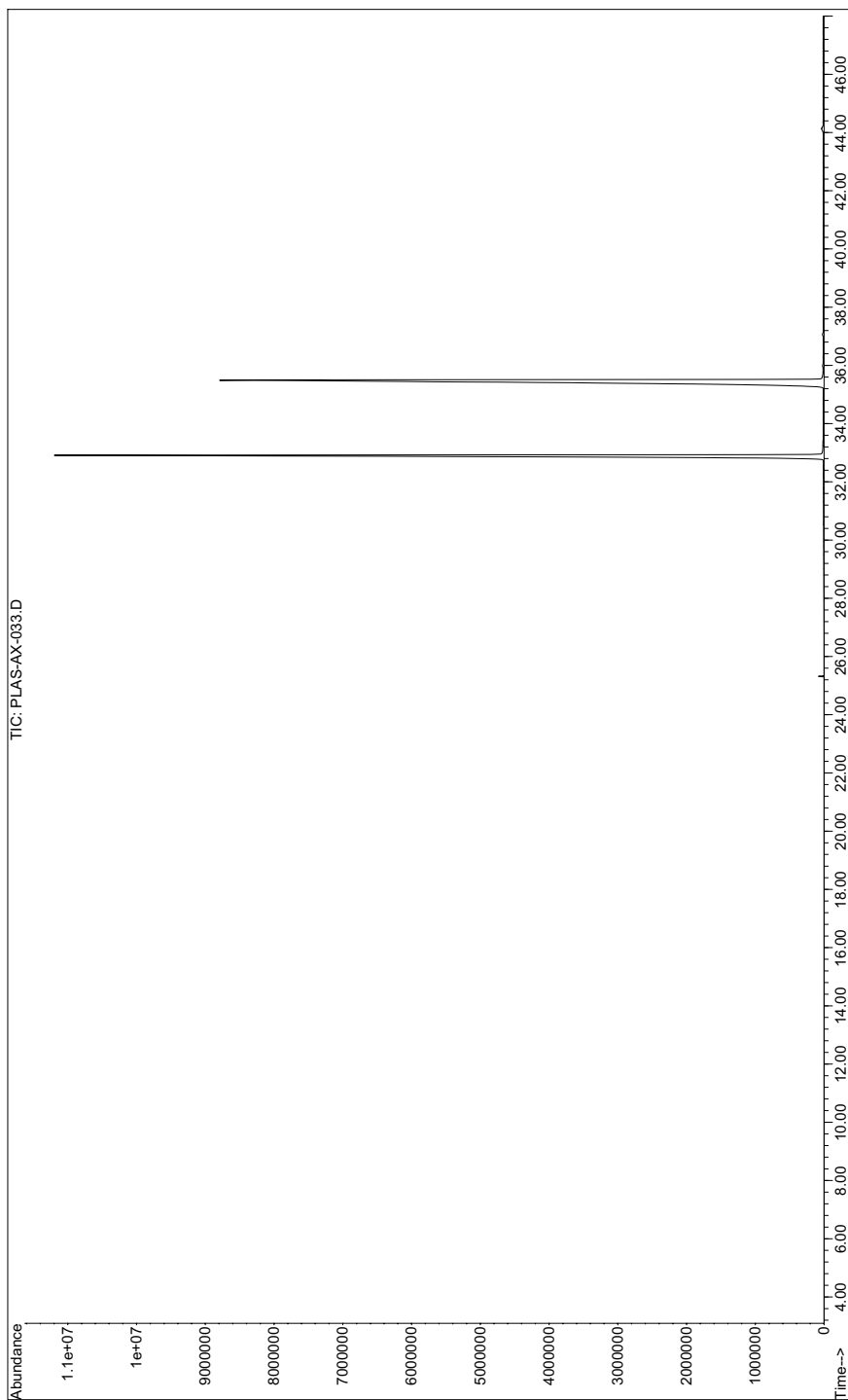
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



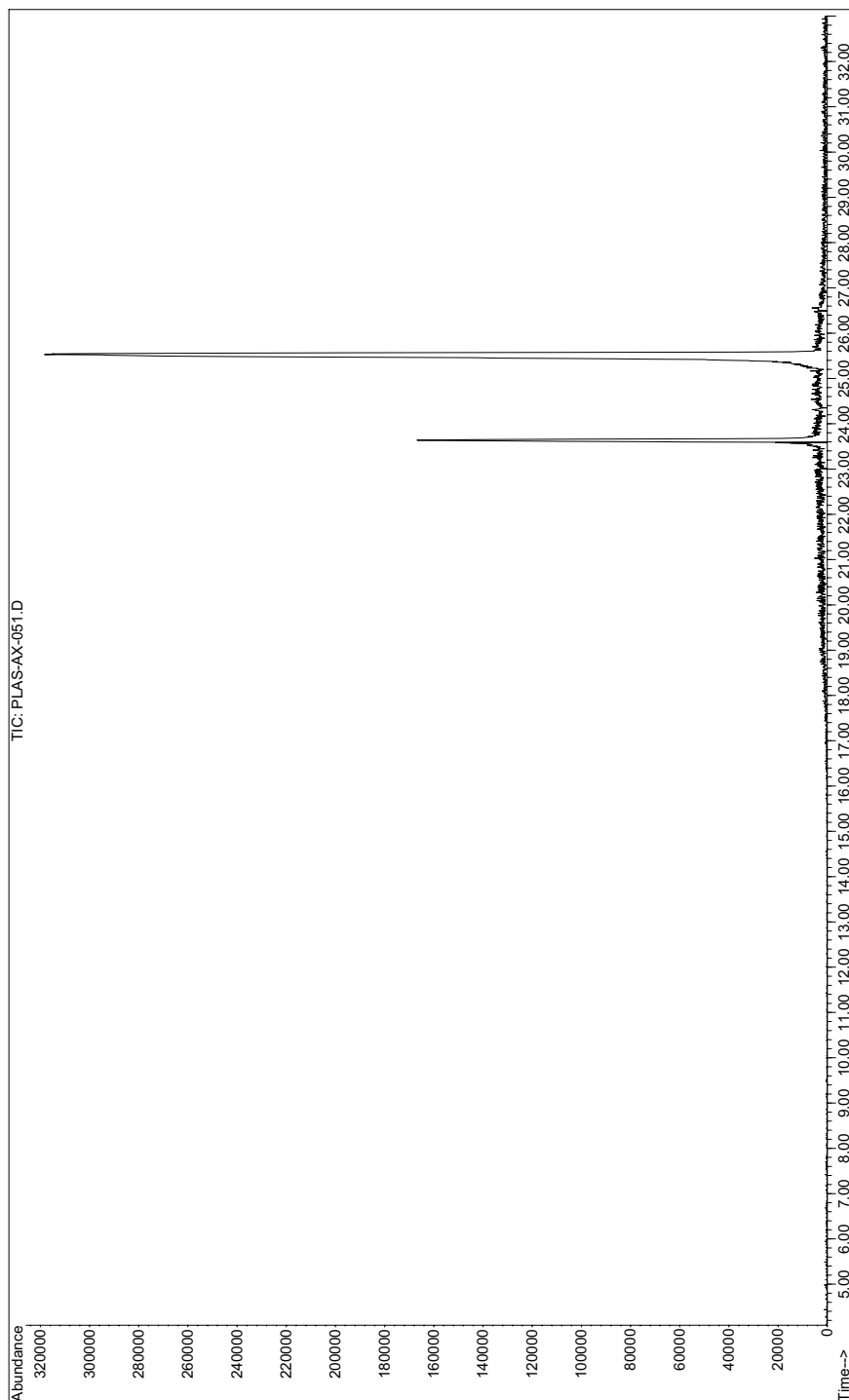
*Analytical Information***Chromatogram for Naugard[®] A - PLAS-AX-026****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for Naugard[®] B-25 - PLAS-AX-061****Analytical Conditions Summary** 40 °C (0 min) to 320 °C (10 min) @ 10 °C/min Det=MSD

*Analytical Information***Chromatogram for Naugard[®] BHT - PLAS-AX-017****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

*Analytical Information***Chromatogram for** *Naugard*[®] *HM-22 - PLAS-AX-033***Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

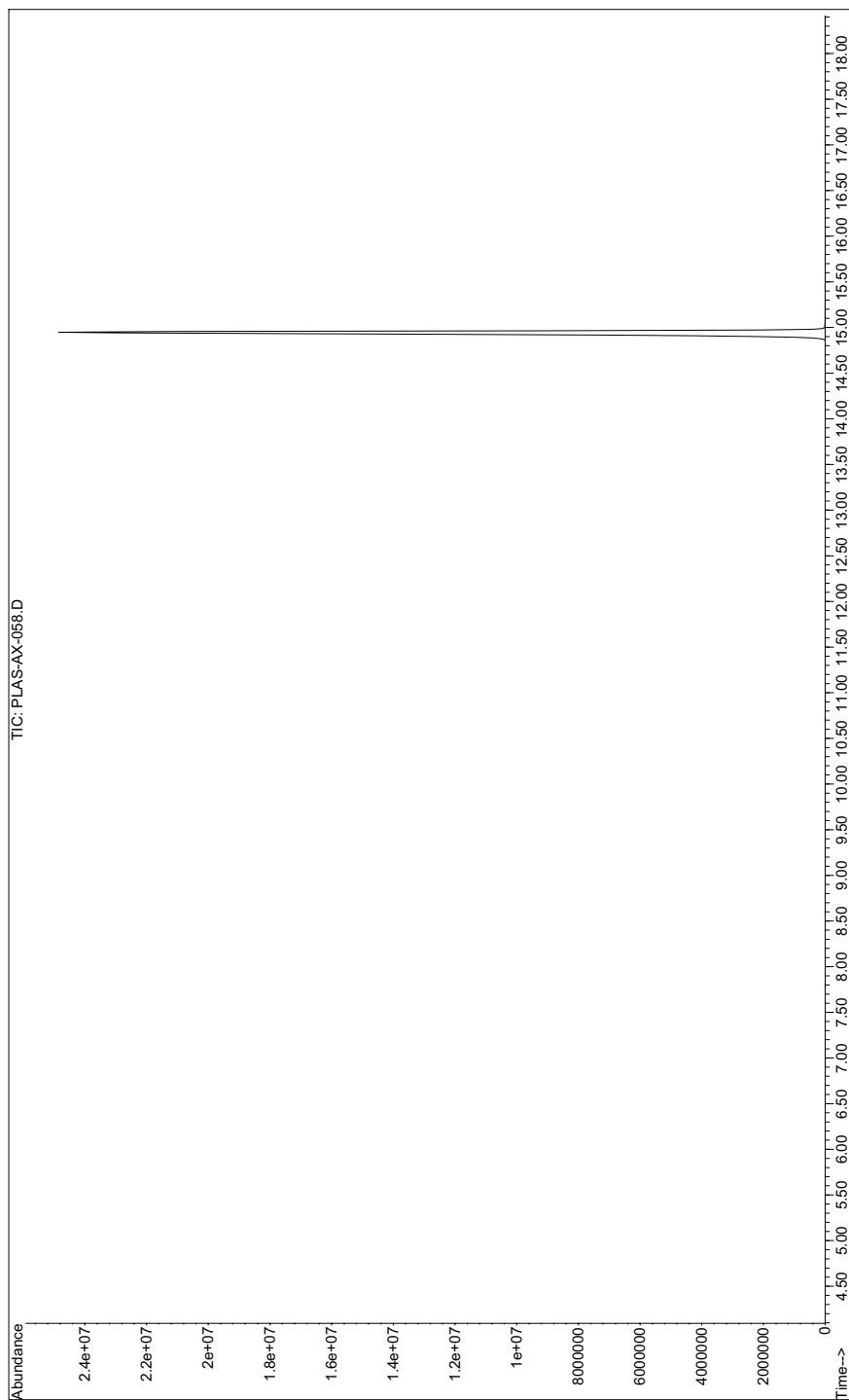
*Analytical Information***Chromatogram for Naugard[®] J - PLAS-AX-048****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

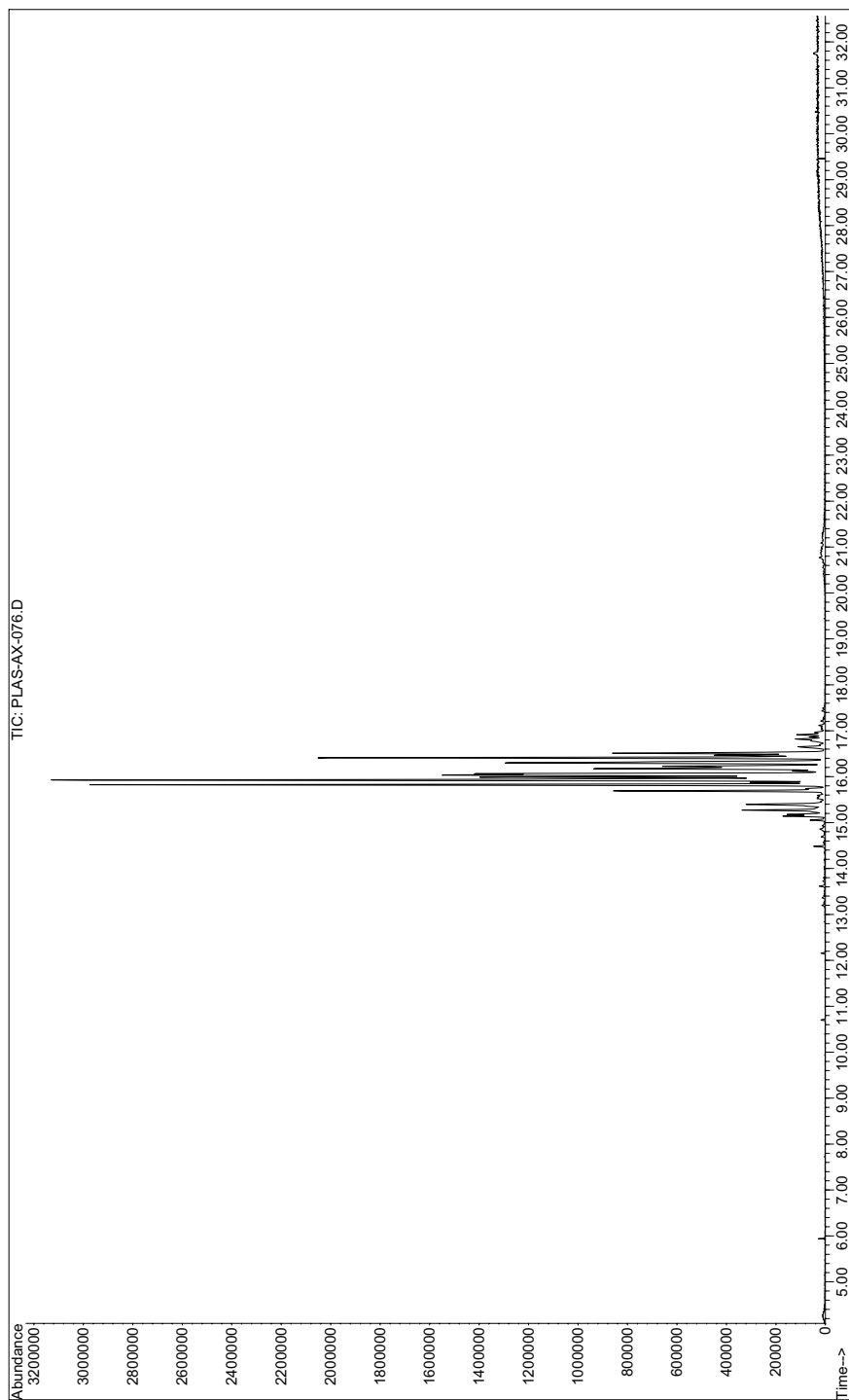
*Analytical Information***Chromatogram for** *Naugard*[®] *NBC - PLAS-AX-051***Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD

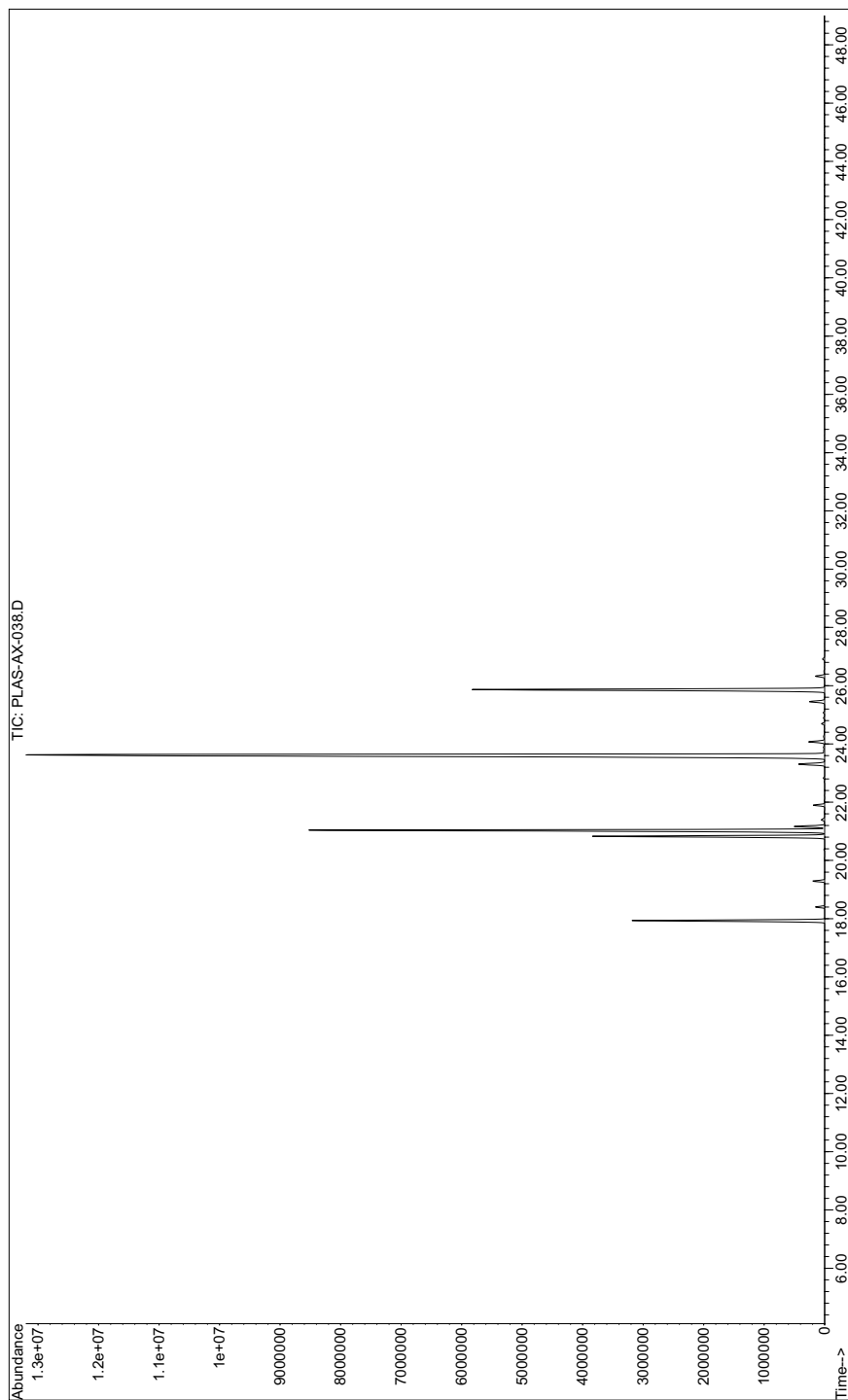
Analytical Information

Chromatogram for Naugard[®] PANA - PLAS-AX-058

Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD



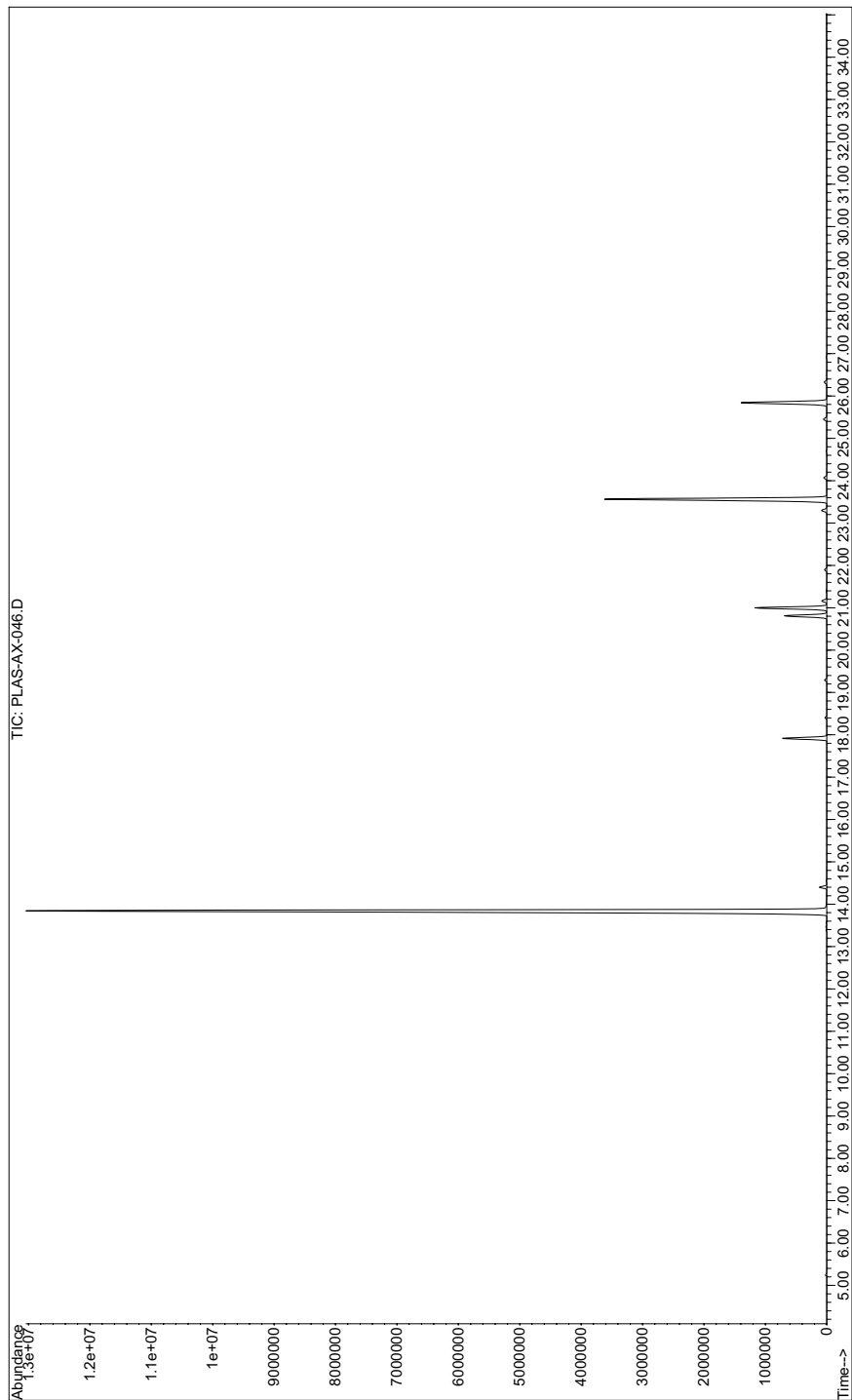
*Analytical Information***Chromatogram for Naugard[®] PHR - PLAS-AX-076****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

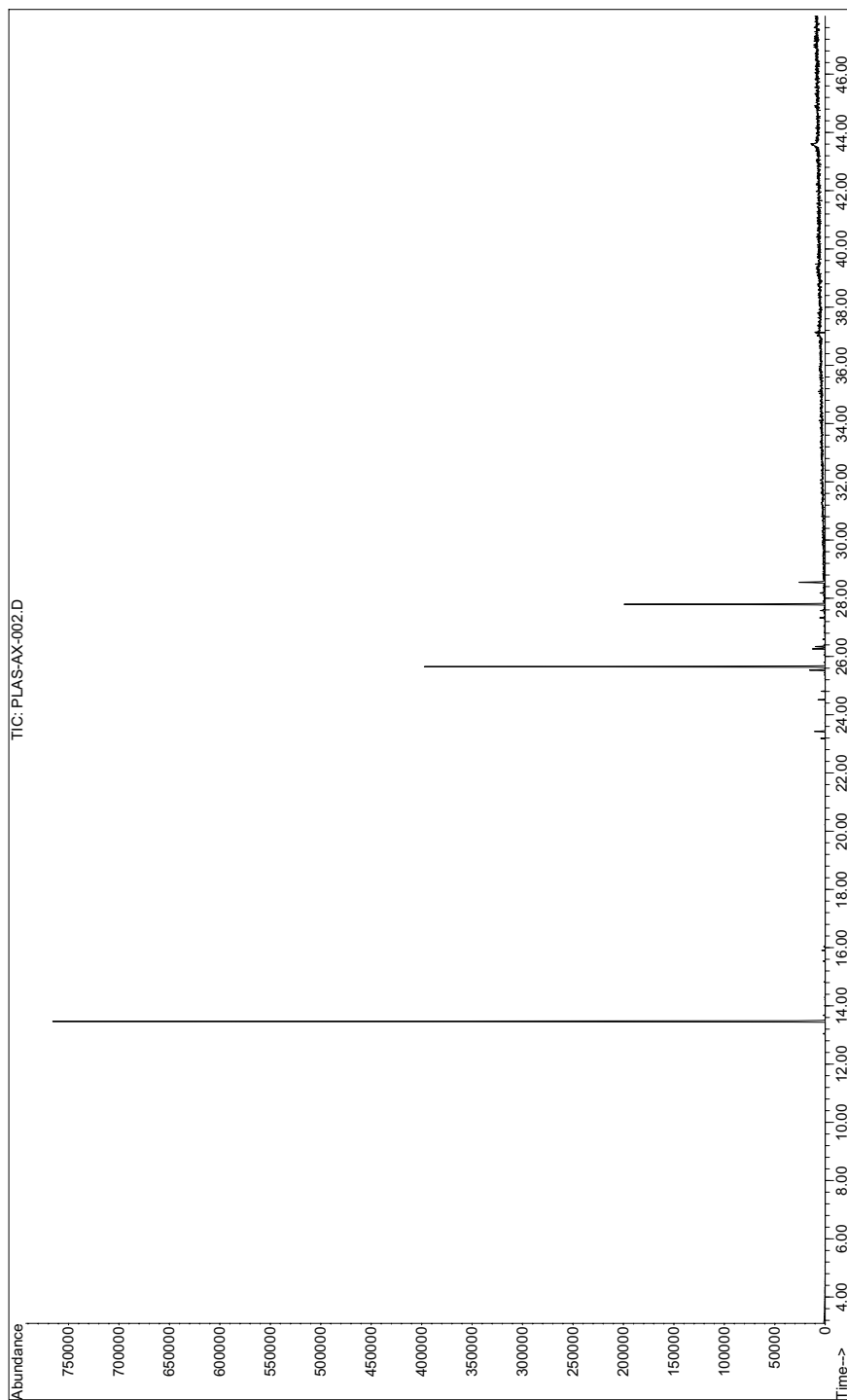
*Analytical Information***Chromatogram for Naugard® PS-30 - PLAS-AX-038****Analytical Conditions Summary** 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD

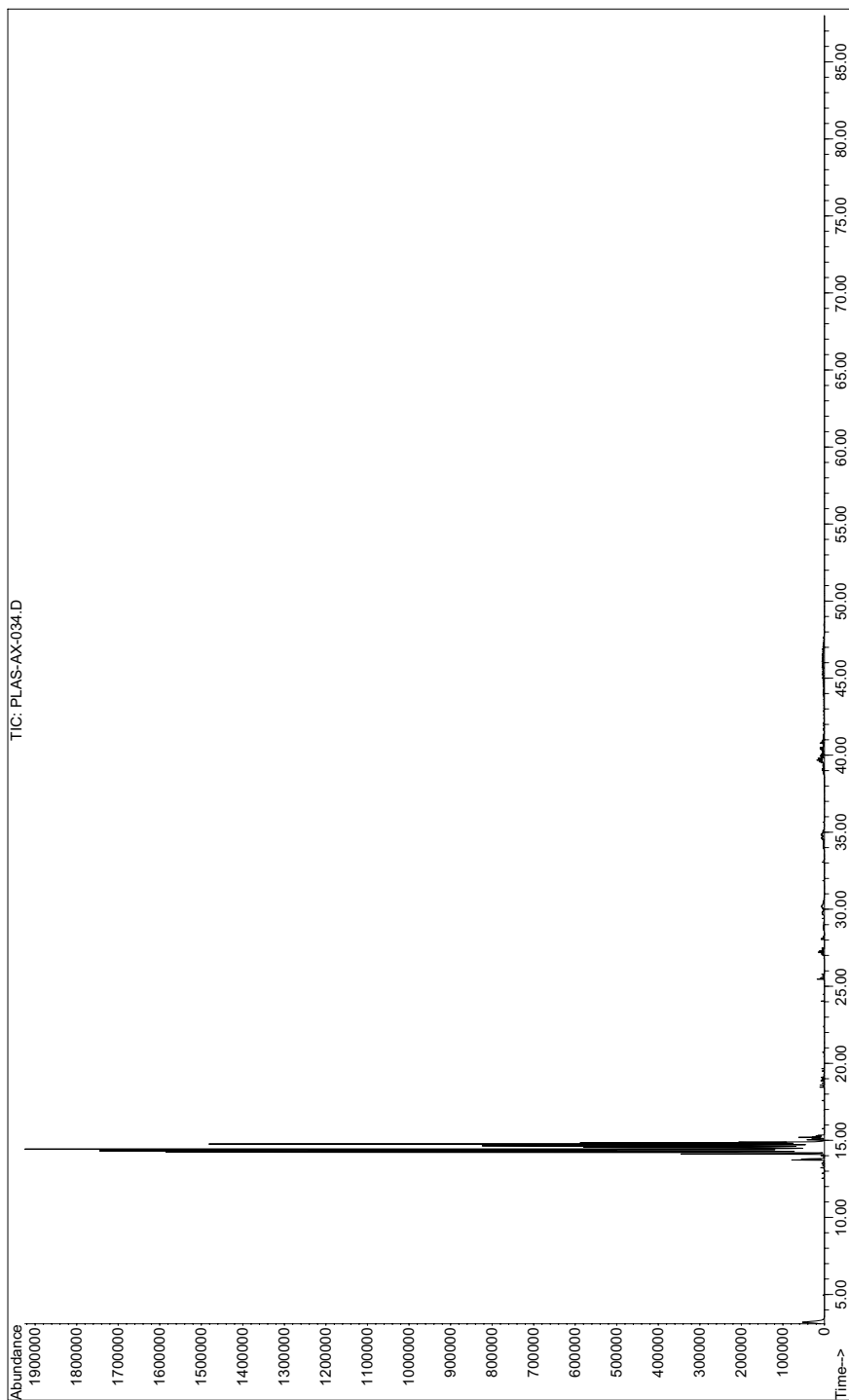
Analytical Information

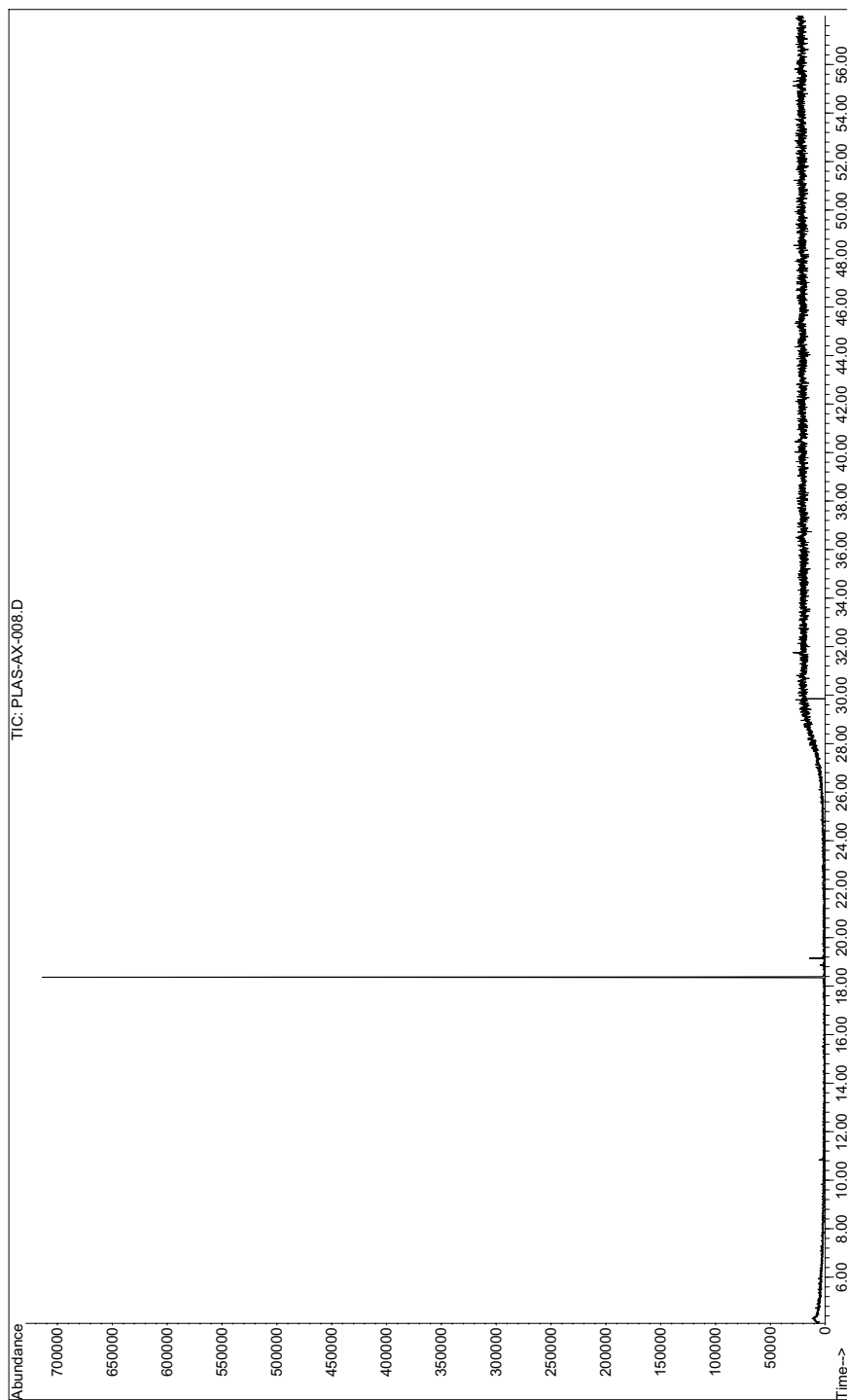
Chromatogram for*Naugard*[®] *PS-35 - PLAS-AX-046*

Analytical Conditions Summary 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD



*Analytical Information***Chromatogram for Naugard[®] Q Extra - PLAS-AX-002****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

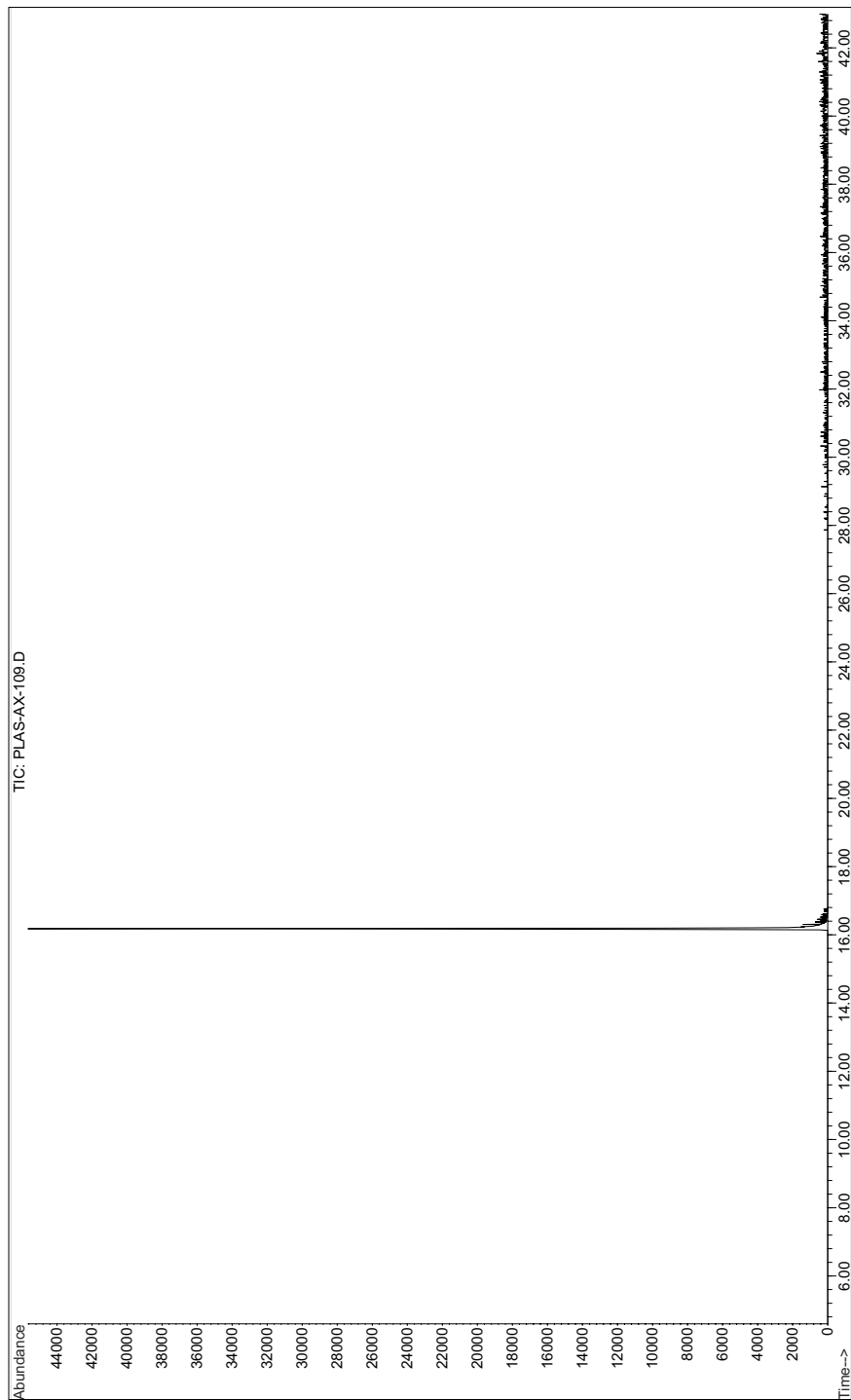
*Analytical Information***Chromatogram for** *Naugard*[®] *RM-51 - PLAS-AX-034***Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

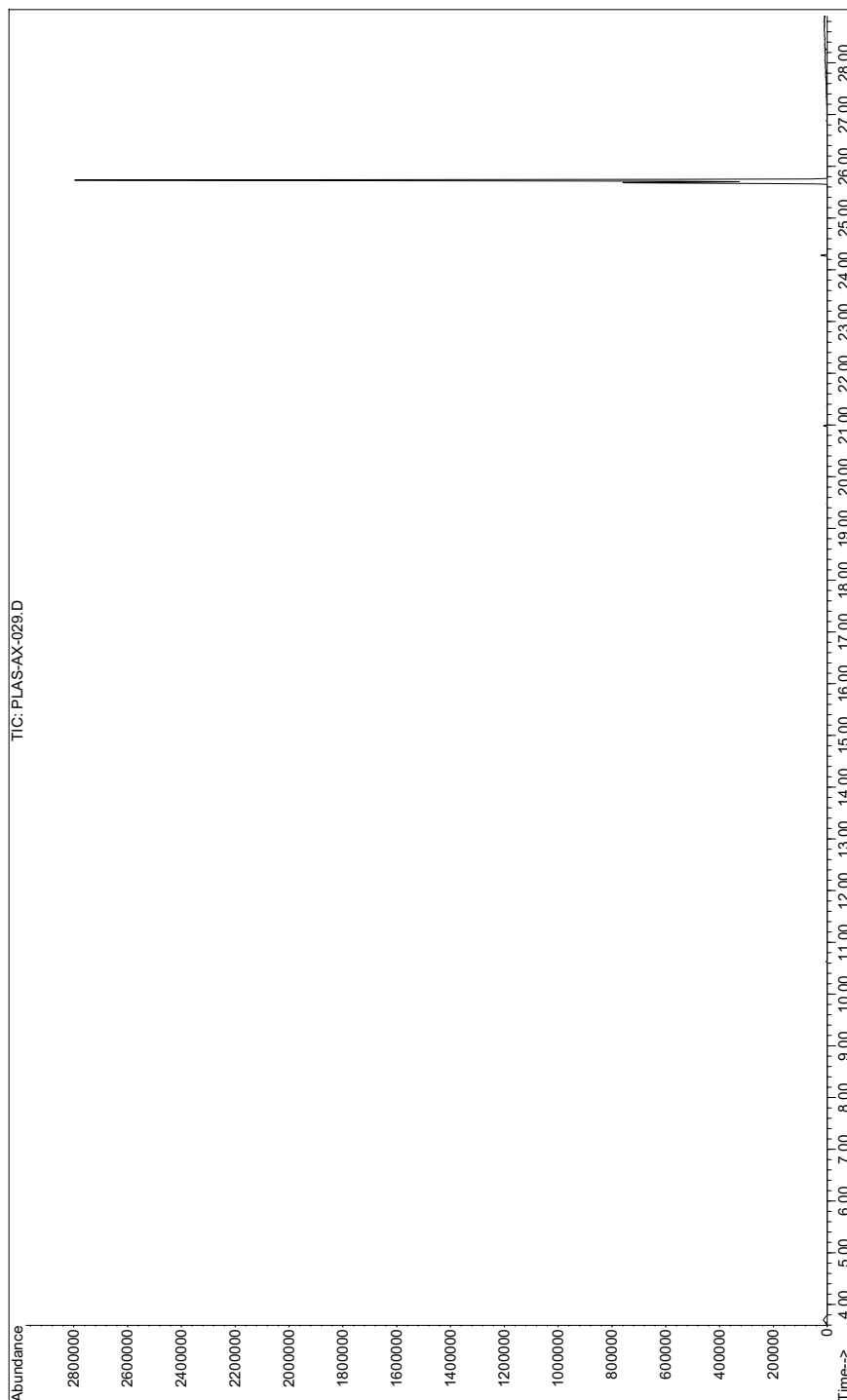
*Analytical Information***Chromatogram for Naugard[®] XL-1 - PLAS-AX-008****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

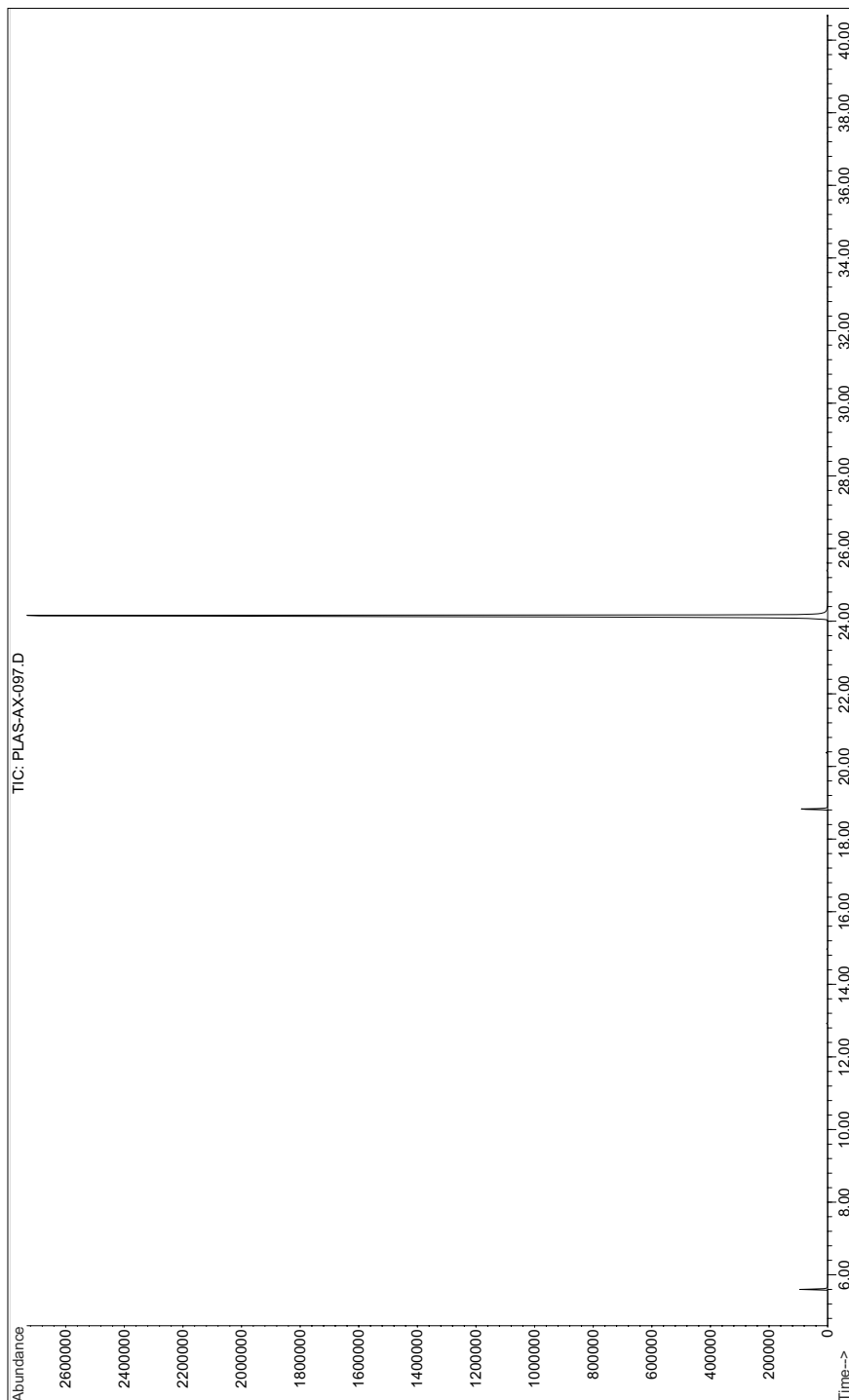
Analytical Information

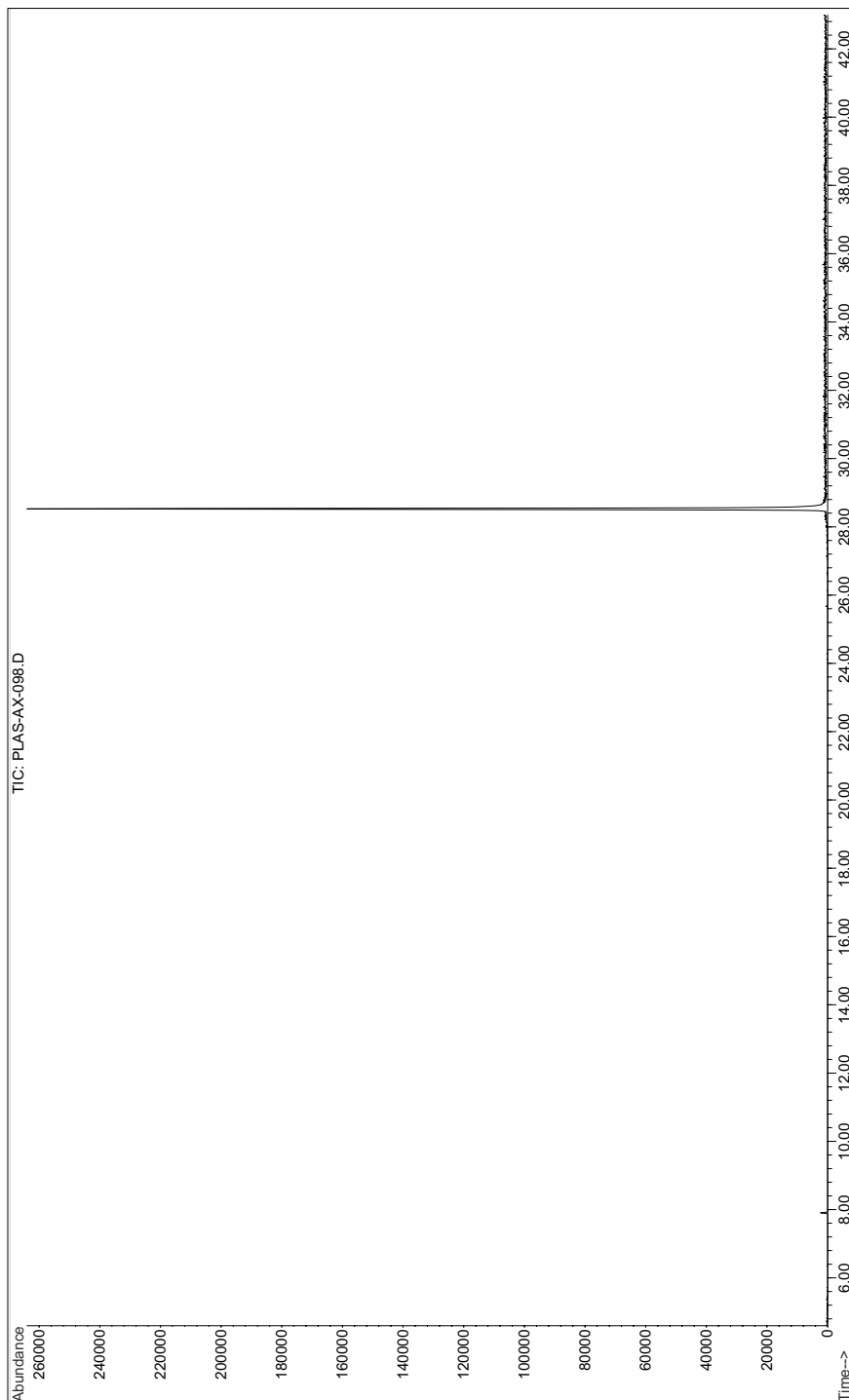
Chromatogram for*Propyl gallate - PLAS-AX-109*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for Santicizer® 278 - PLAS-AX-029****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

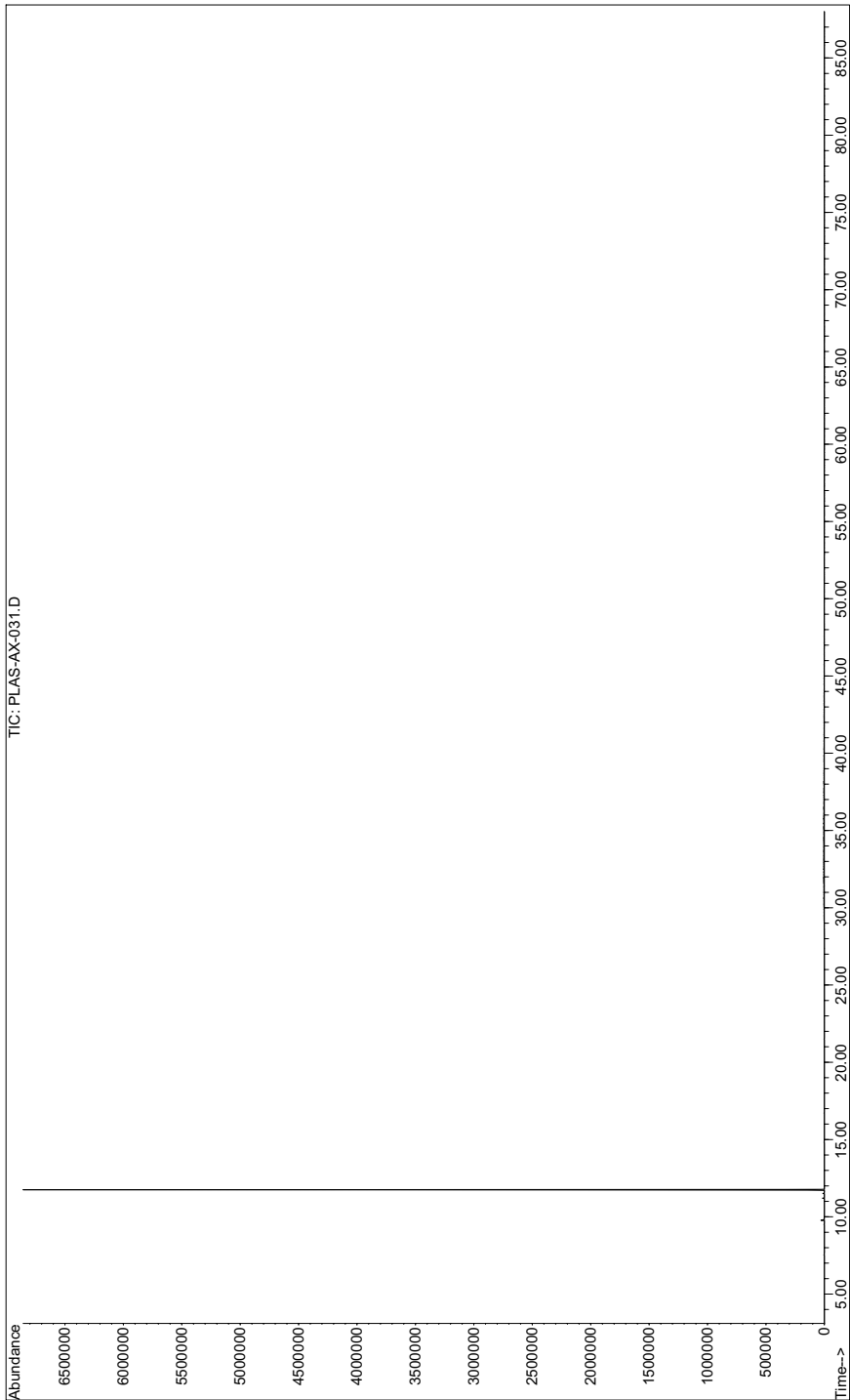
*Analytical Information***Chromatogram for *Bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate* - PLAS-AX-097****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for 2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole) - PLAS-AX-098****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

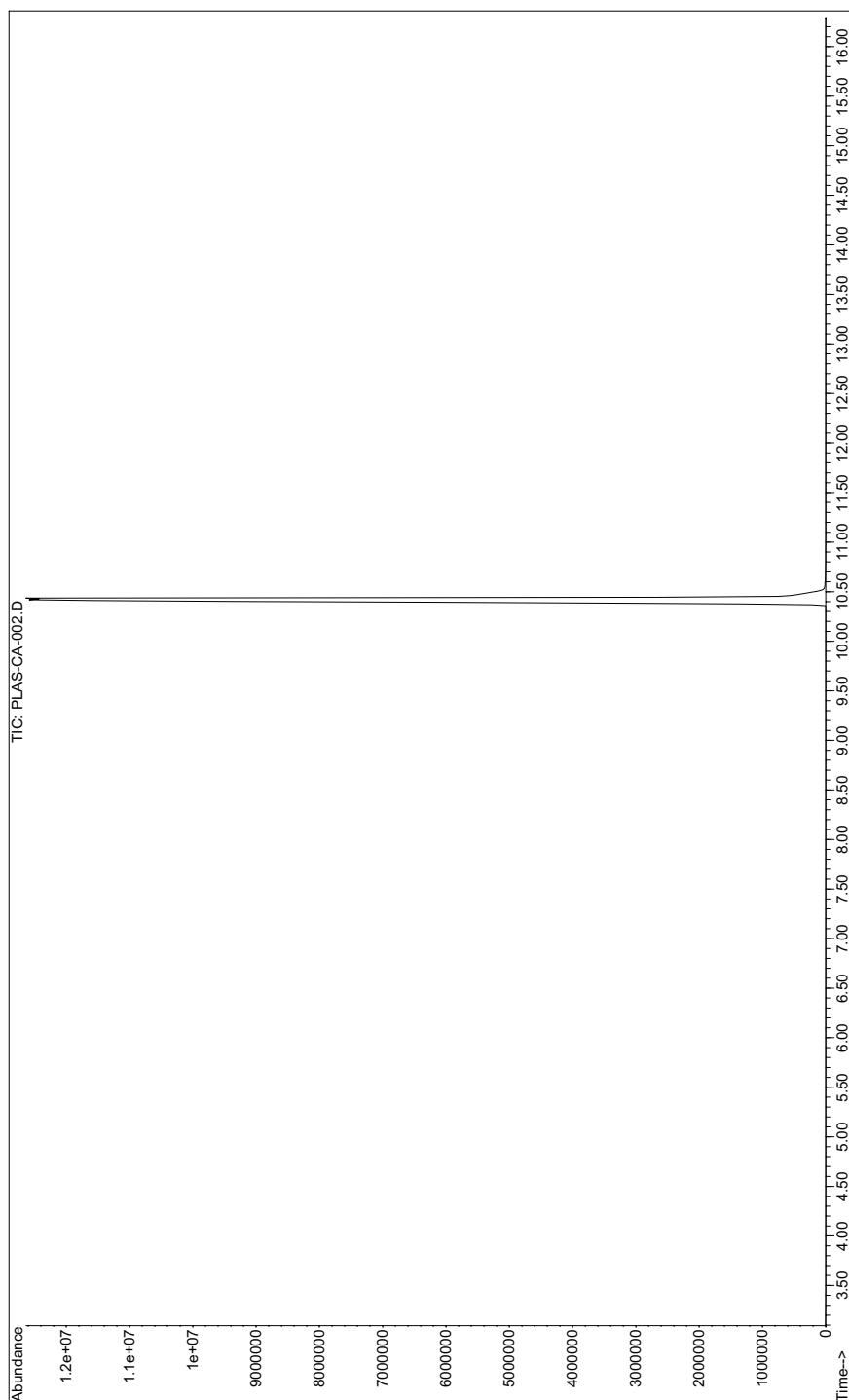
Chromatogram for *Ultrinox*[®] 626 - PLAS-AX-031

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *Silquest*[®] A-1100 - PLAS-CA-002****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

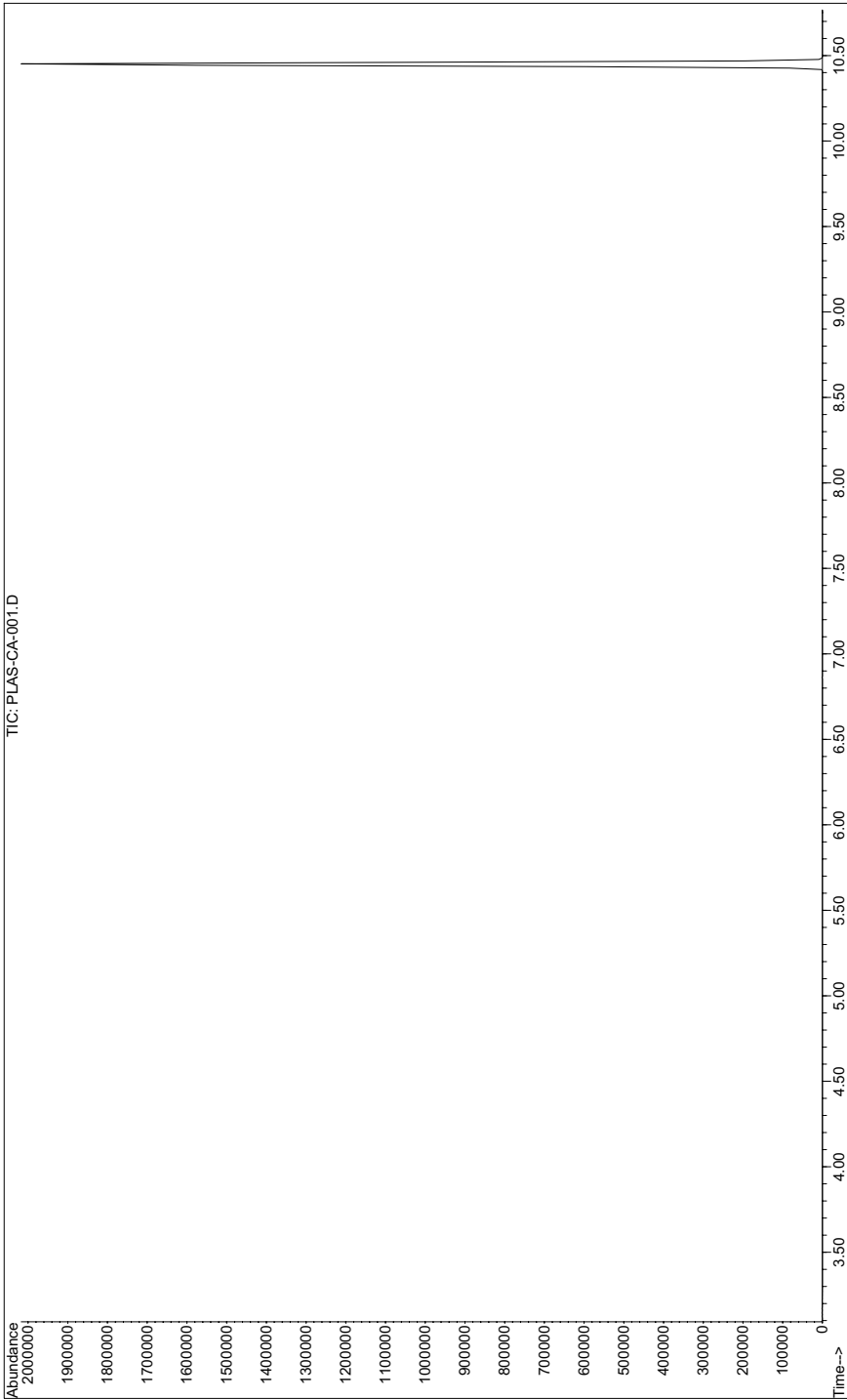
Inj Temp=250 °C, Det=MSD



Analytical Information

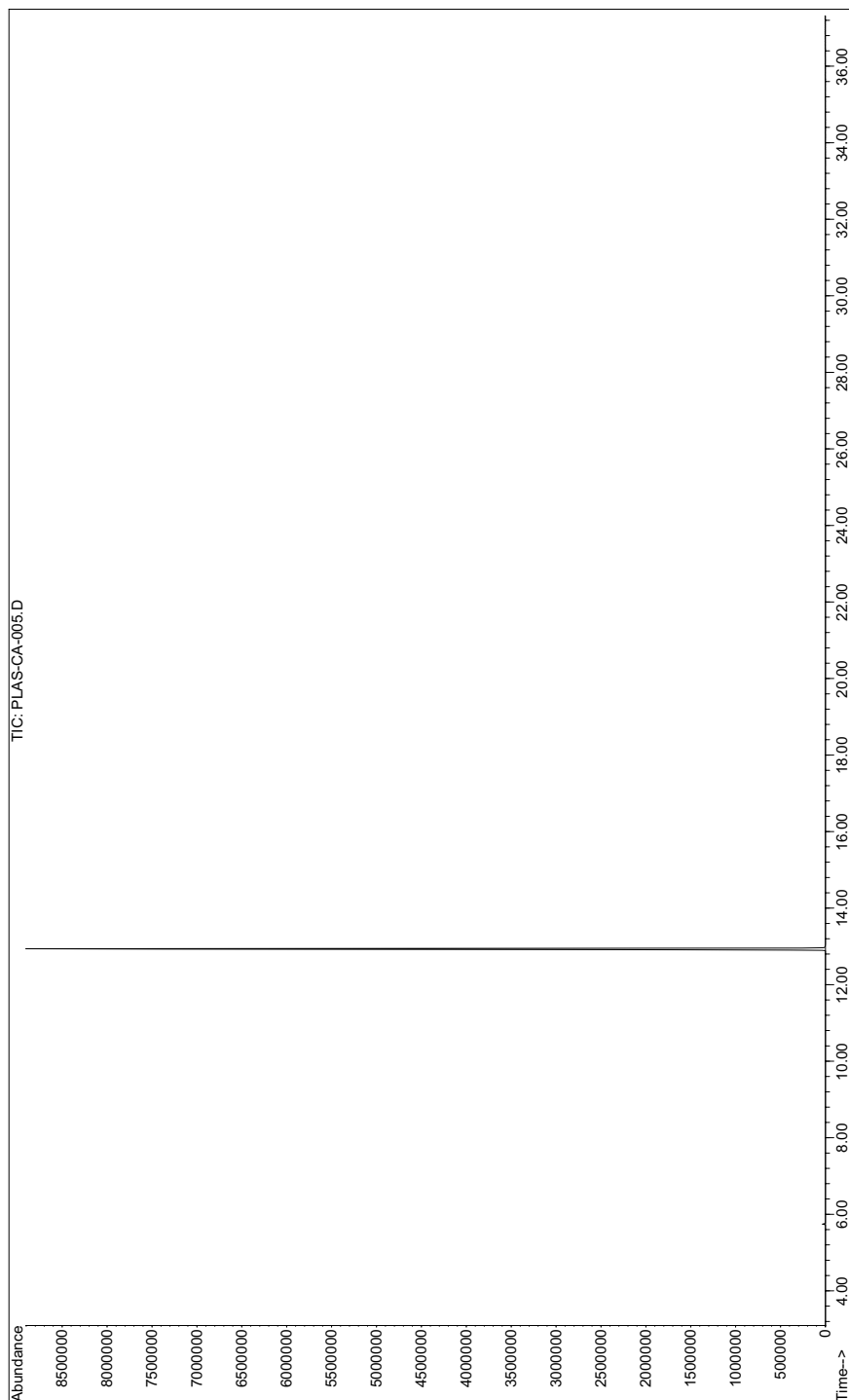
Chromatogram for *Silquest® A-1289 - PLAS-CA-001*

Analytical Conditions Summary
Temp (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *Silquest*[®] A-137 - PLAS-CA-005****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

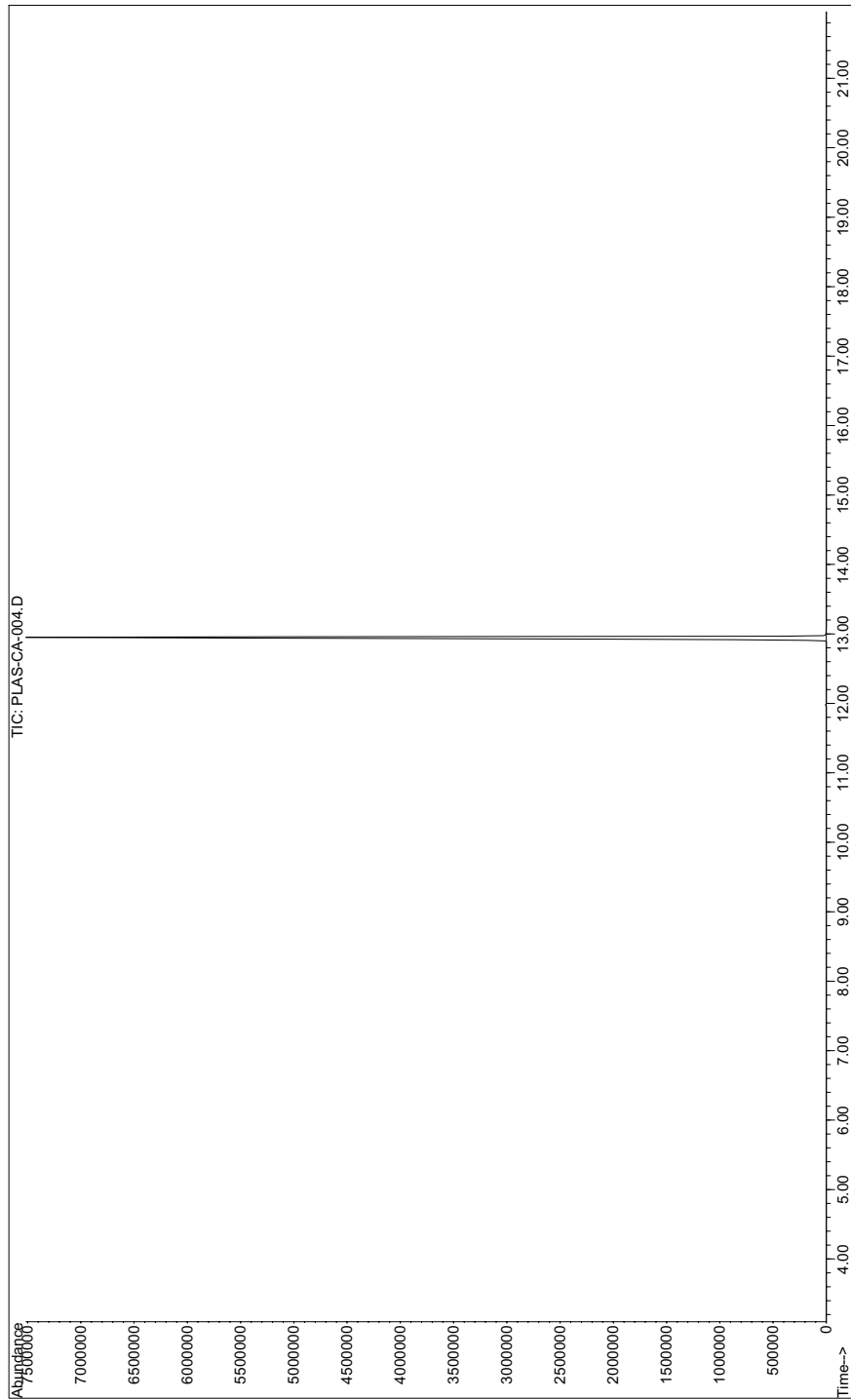
Inj Temp=250 °C, Det=MSD



Analytical Information

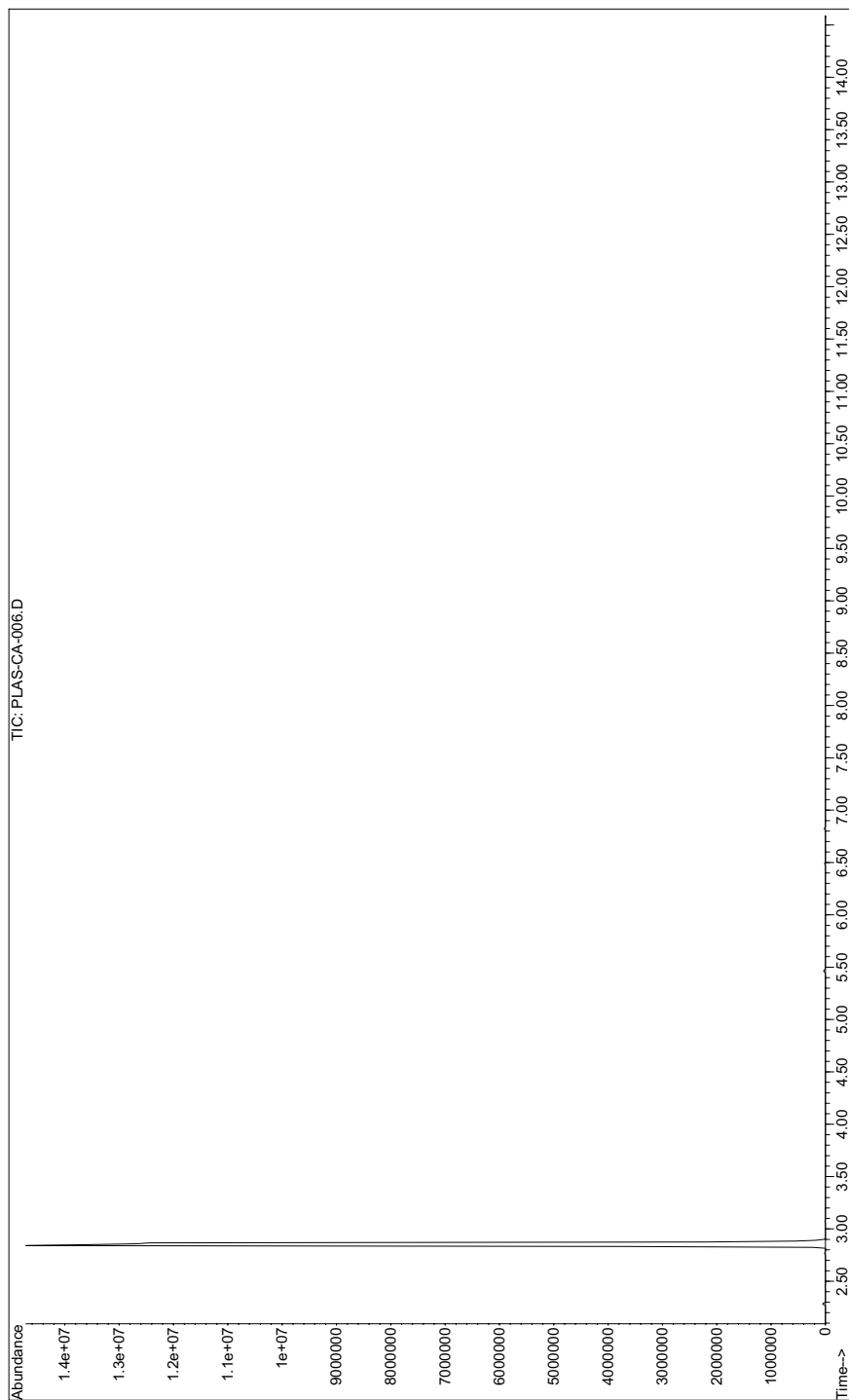
Chromatogram for *Silquest® A-187 - PLAS-CA-004*

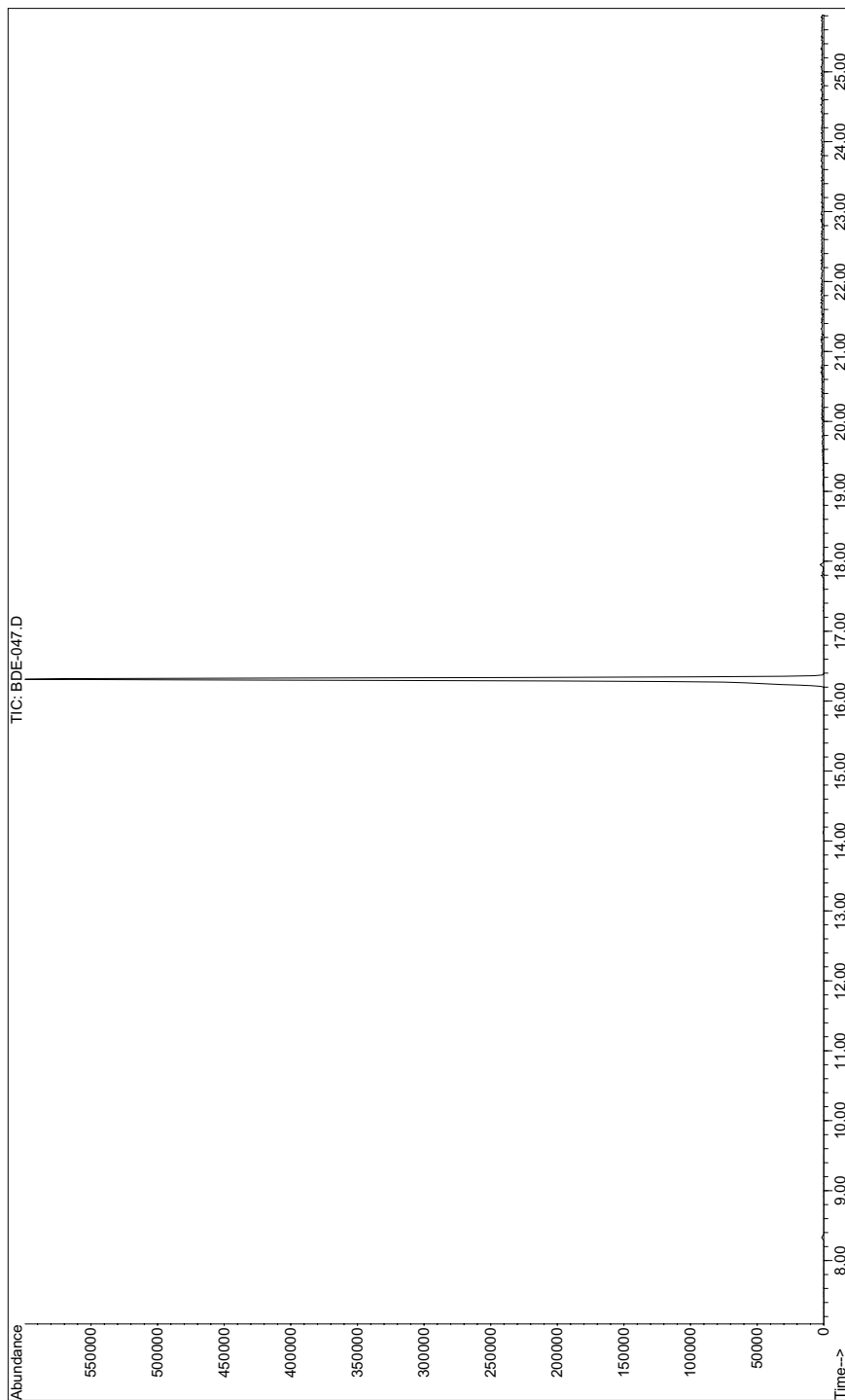
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

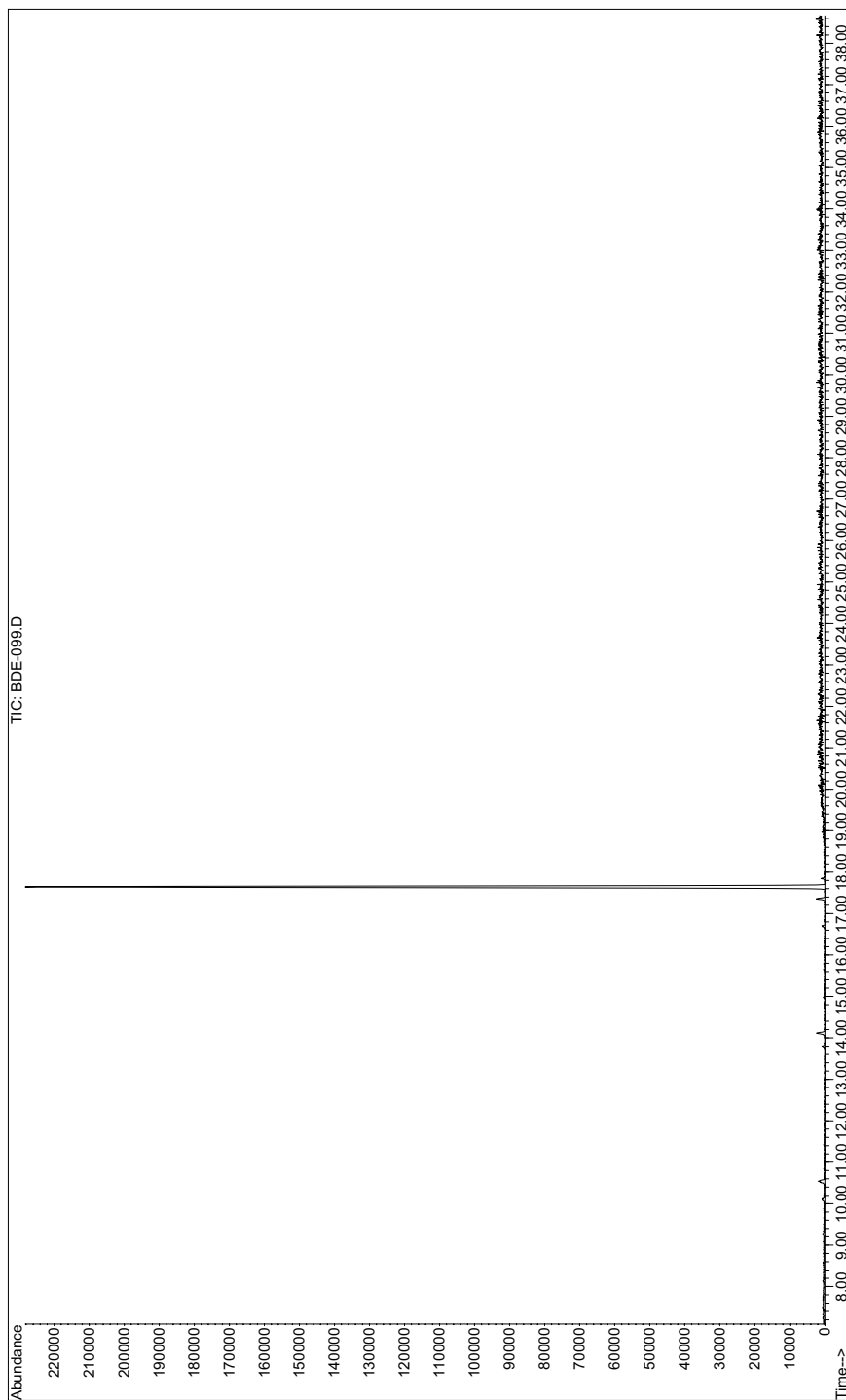


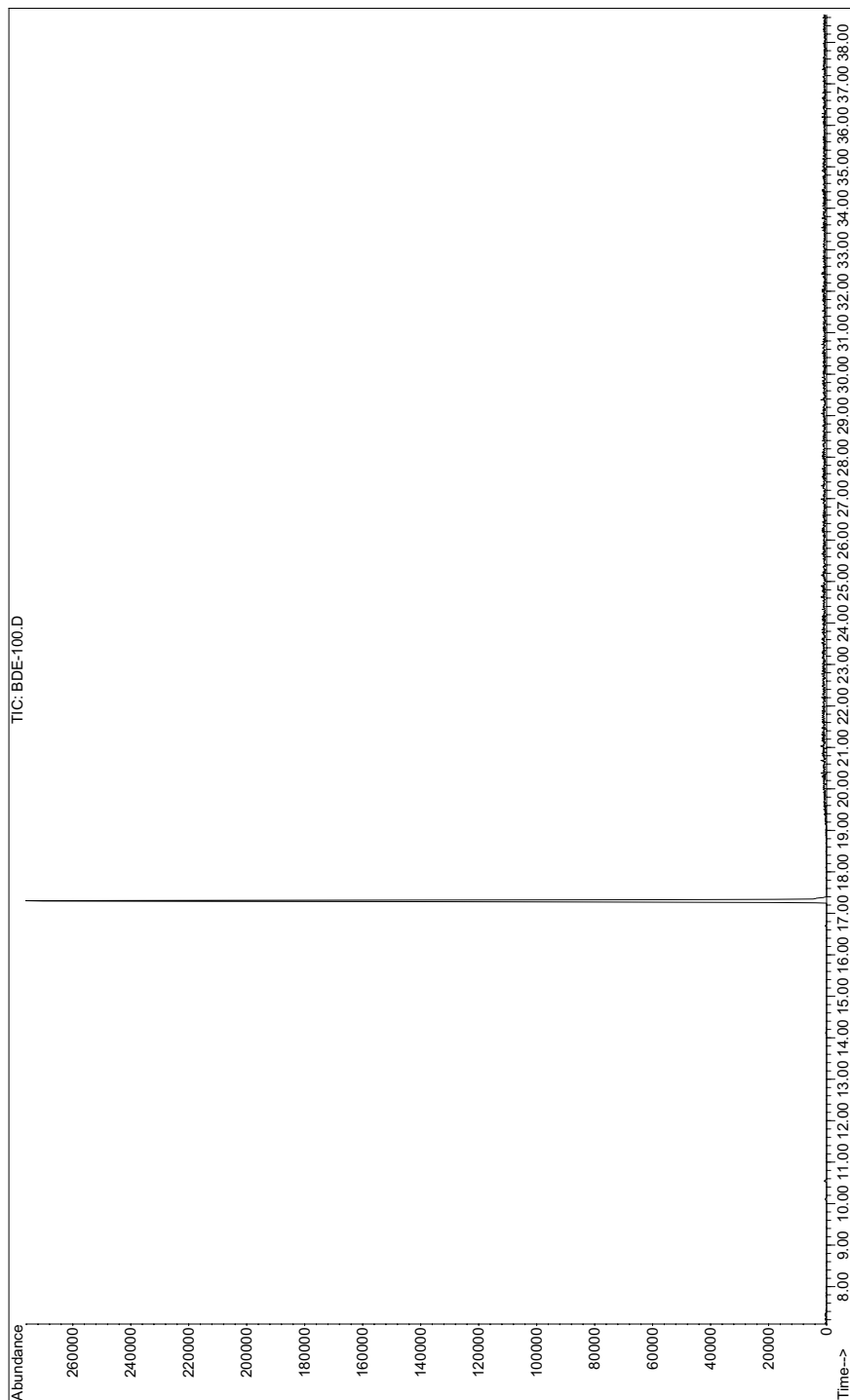
*Analytical Information***Chromatogram for *Silquest*[®] A-2171 - PLAS-CA-006****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

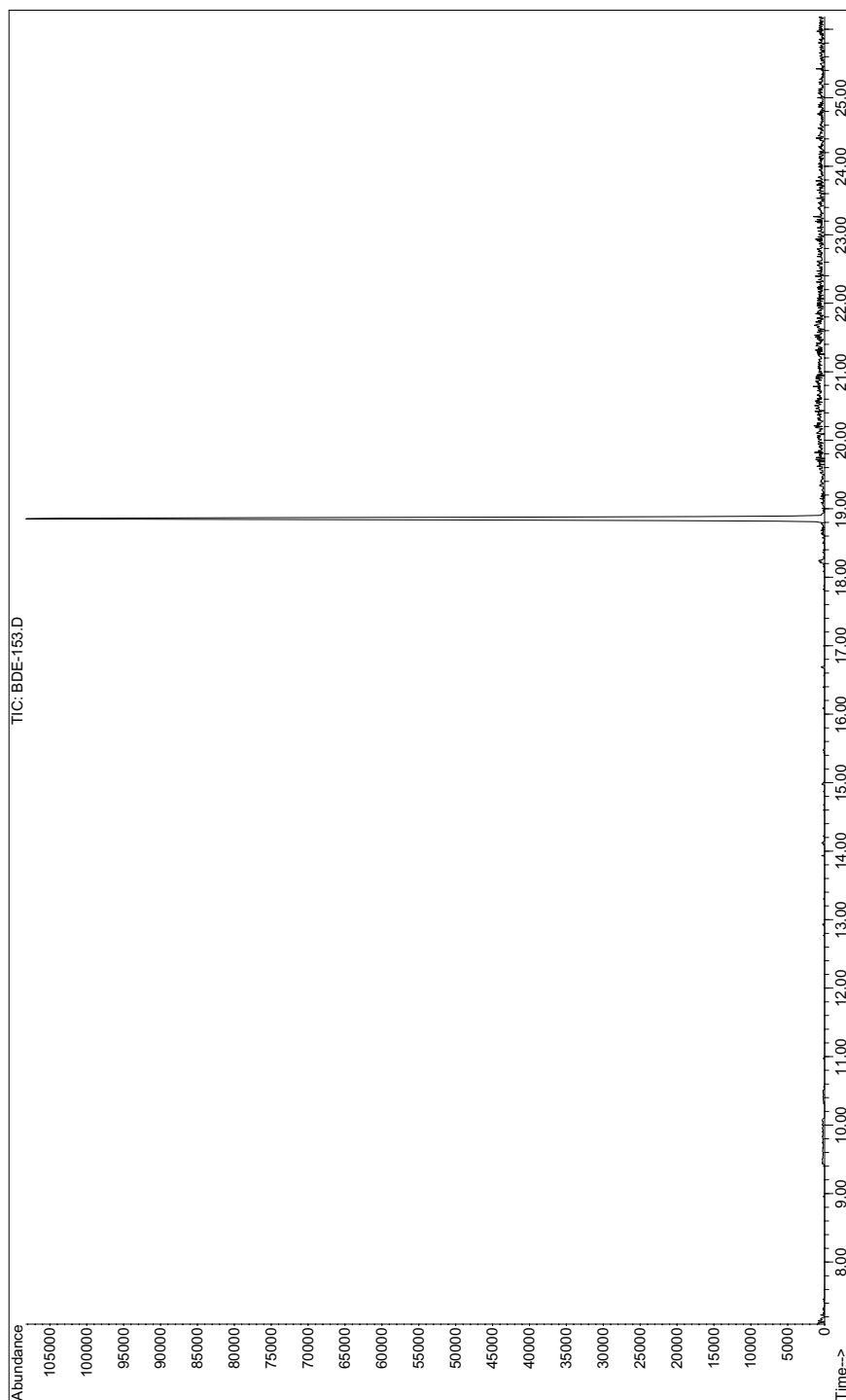
Inj Temp=250 °C, Det=MSD

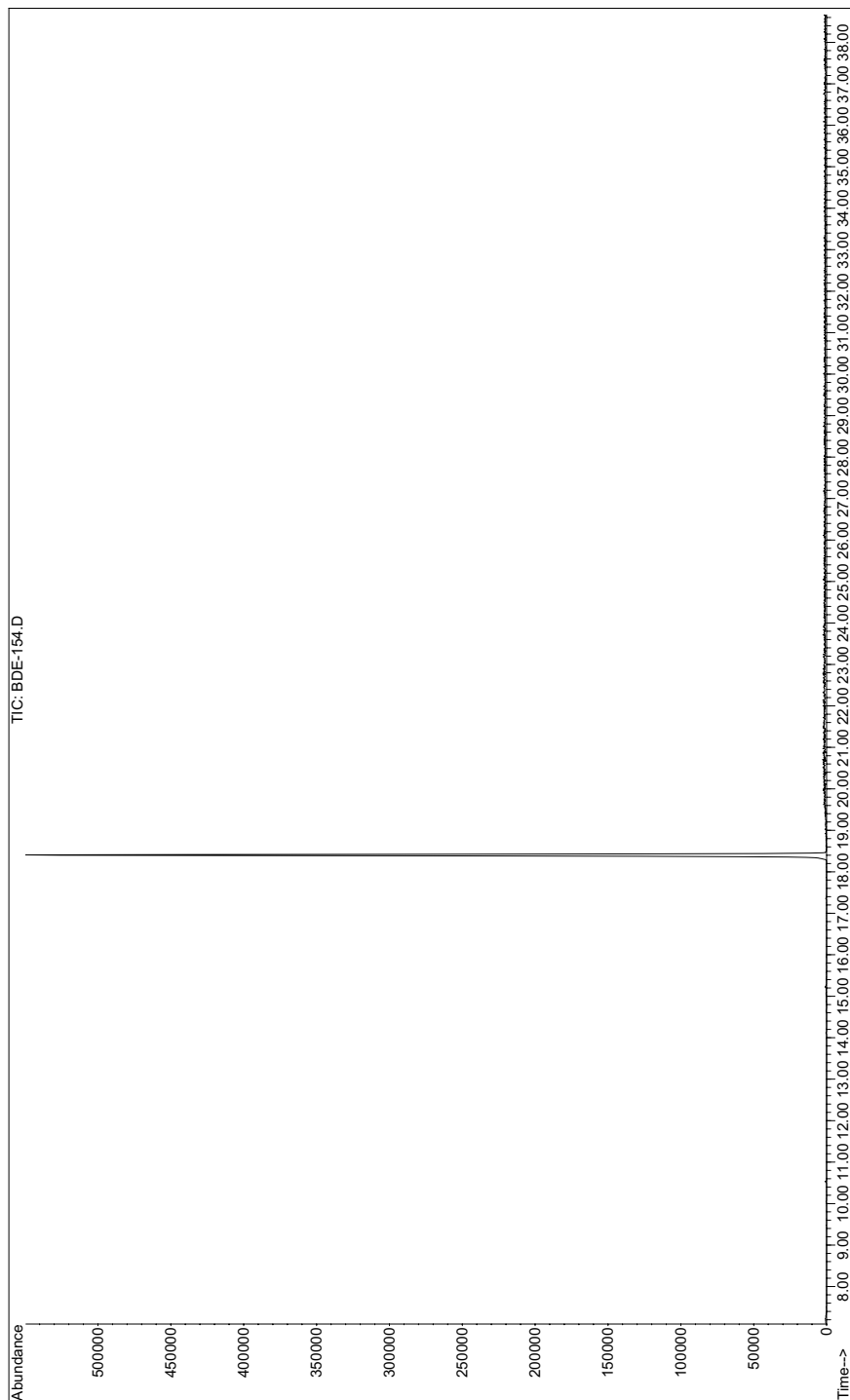


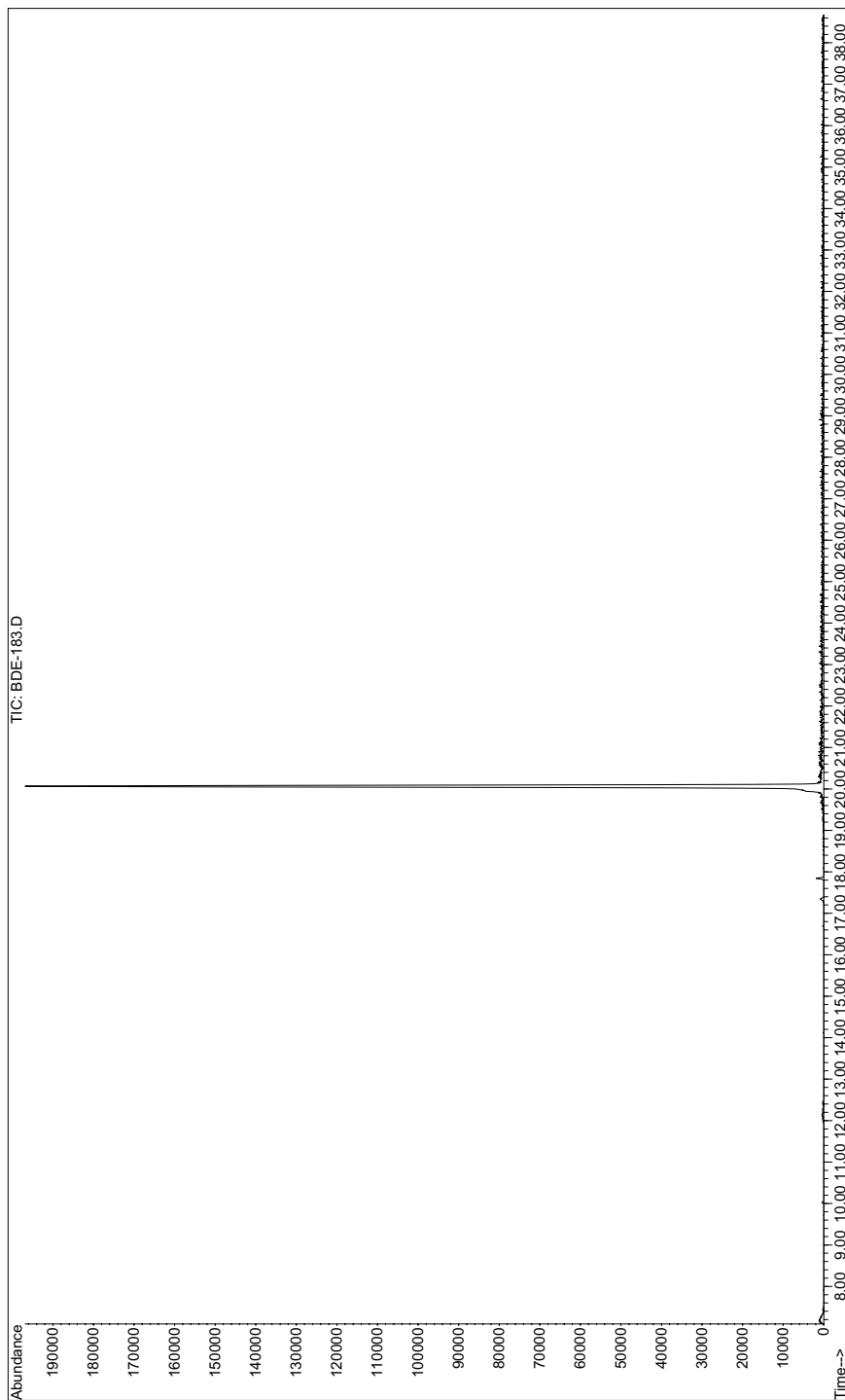
*Analytical Information***Chromatogram for 2,2',4,4'-Tetrabromodiphenyl ether - BDE-047****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

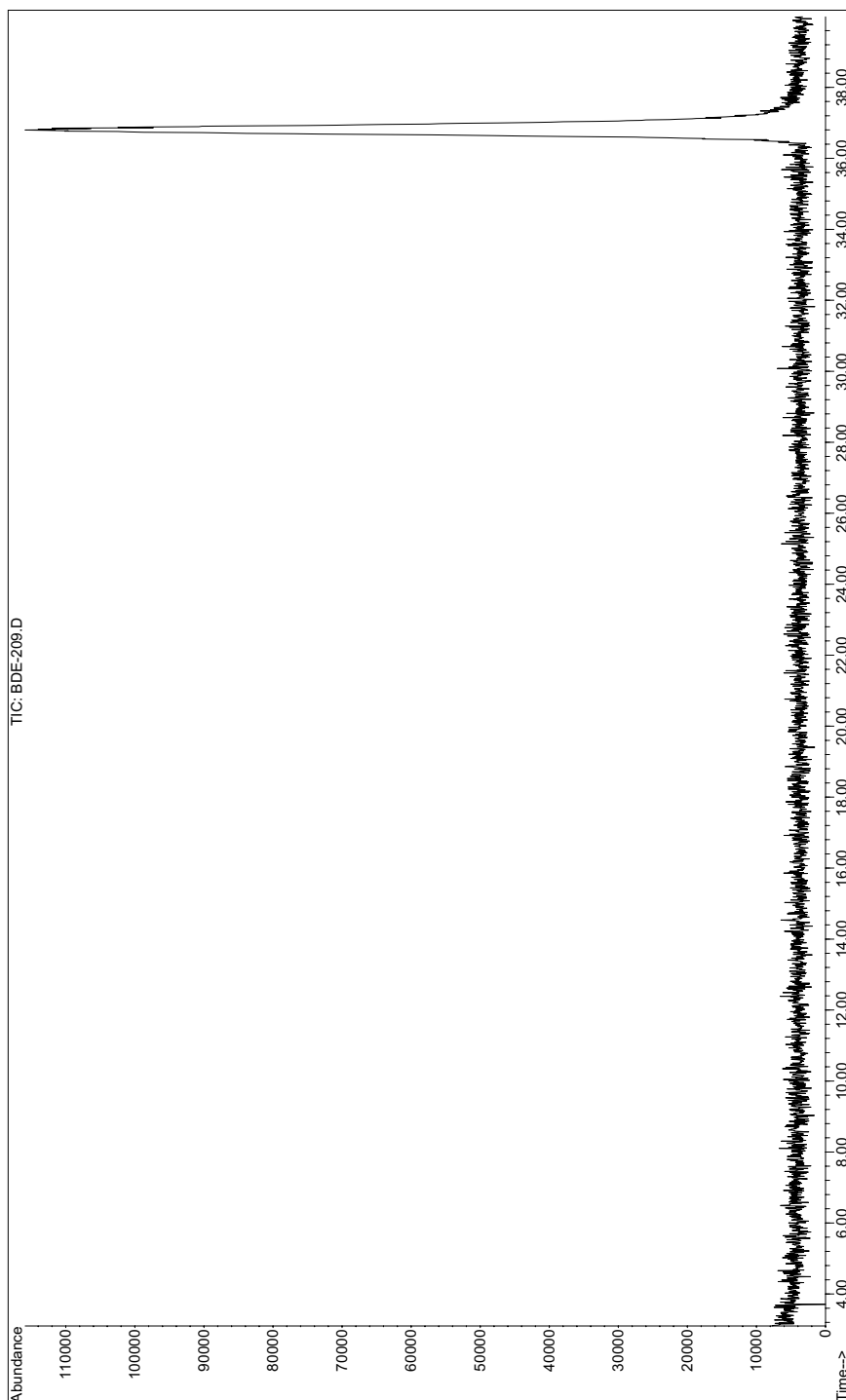
*Analytical Information***Chromatogram for 2,2',4,4',5-Pentabromodiphenyl ether - BDE-099****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

*Analytical Information***Chromatogram for 2,2',4,4',6-Pentabromodiphenyl ether - BDE-100****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

*Analytical Information***Chromatogram for 2,2',4,4',5,5'-Hexabromodiphenyl ether - BDE-153****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

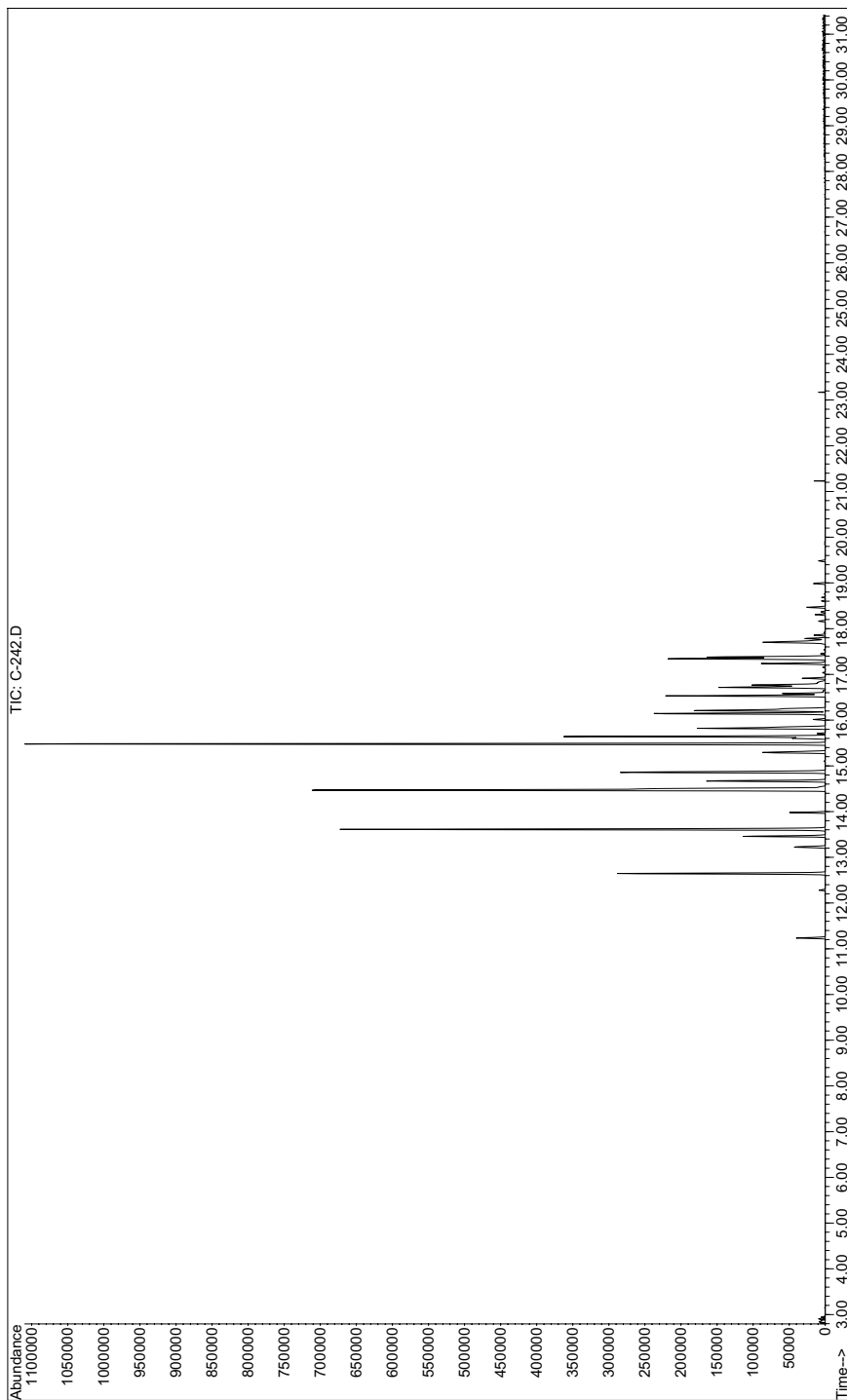
*Analytical Information***Chromatogram for 2,2',4,4',5,6'-Hexabromodiphenyl ether - BDE-154****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

*Analytical Information***Chromatogram for 2,2',3,4,4',5',6-Heptabromodiphenyl ether - BDE-183****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

*Analytical Information***Chromatogram for Decabromodiphenyl ether - BDE-209****Analytical Conditions Summary** 200°C (1min) to 340°C (10min) @ 40°C/min Det=MSD

*Analytical Information***Chromatogram for Aroclor®1242 - C-242****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

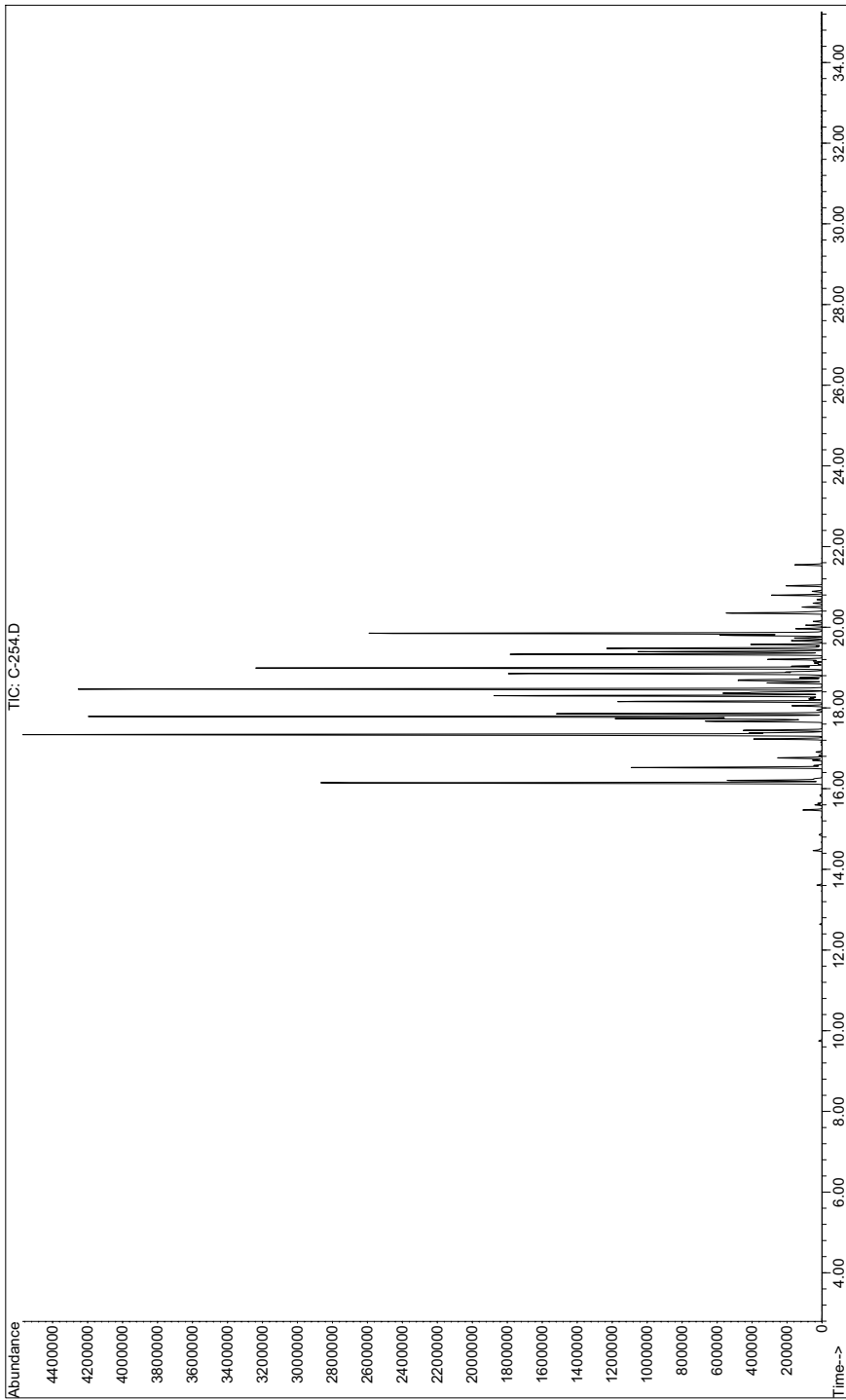
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Aroclor® 1254 - C-254

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

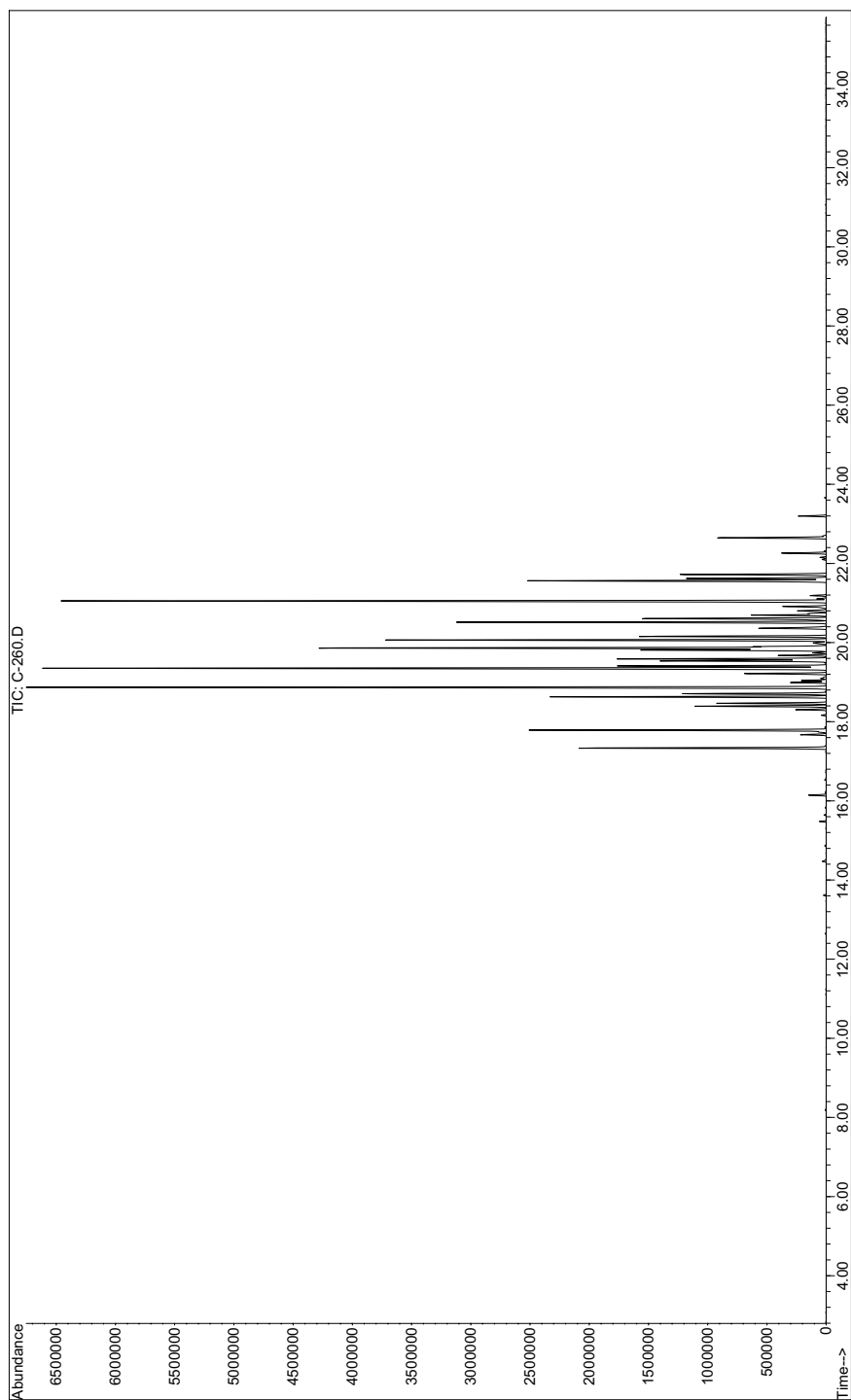


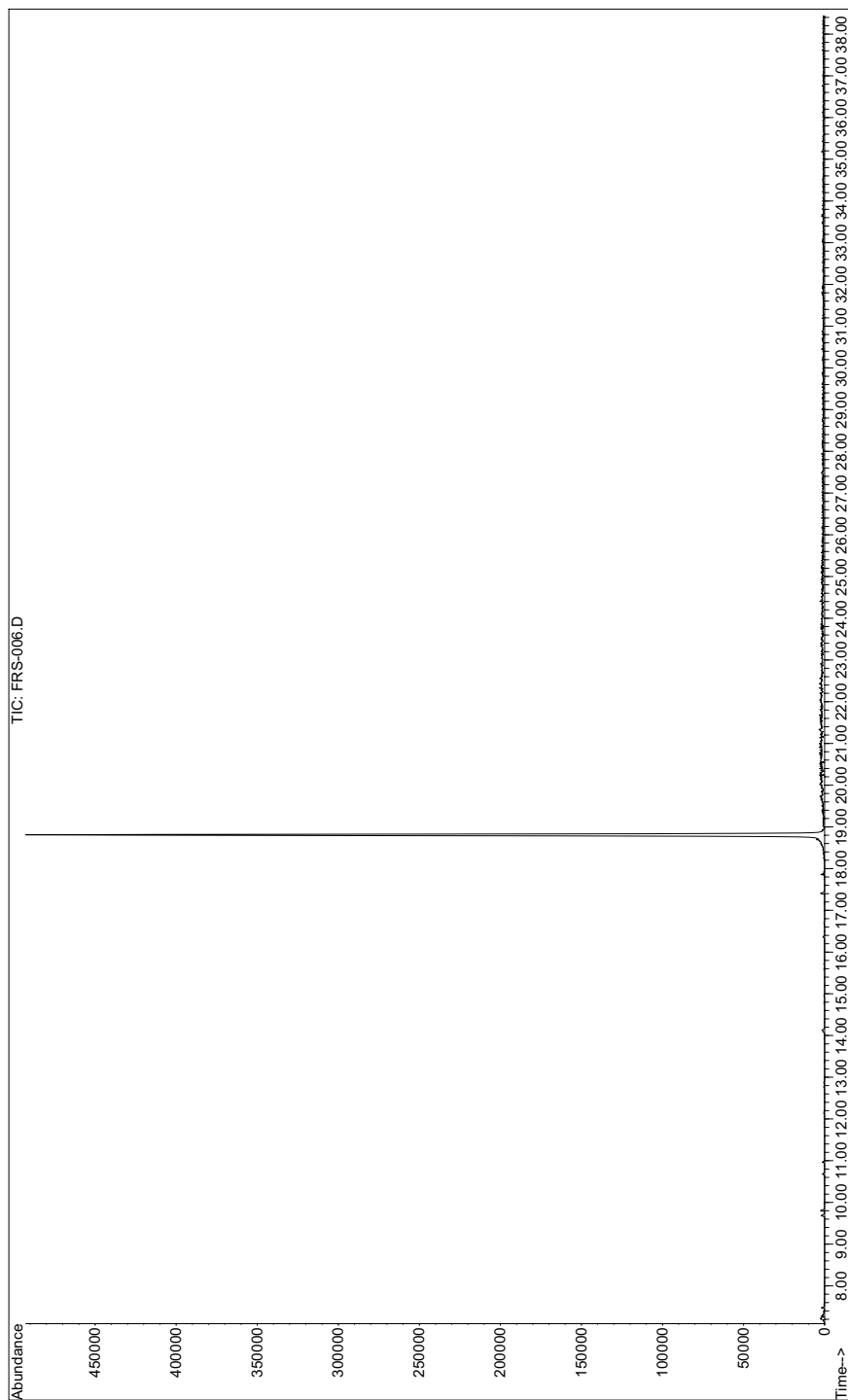
Analytical Information

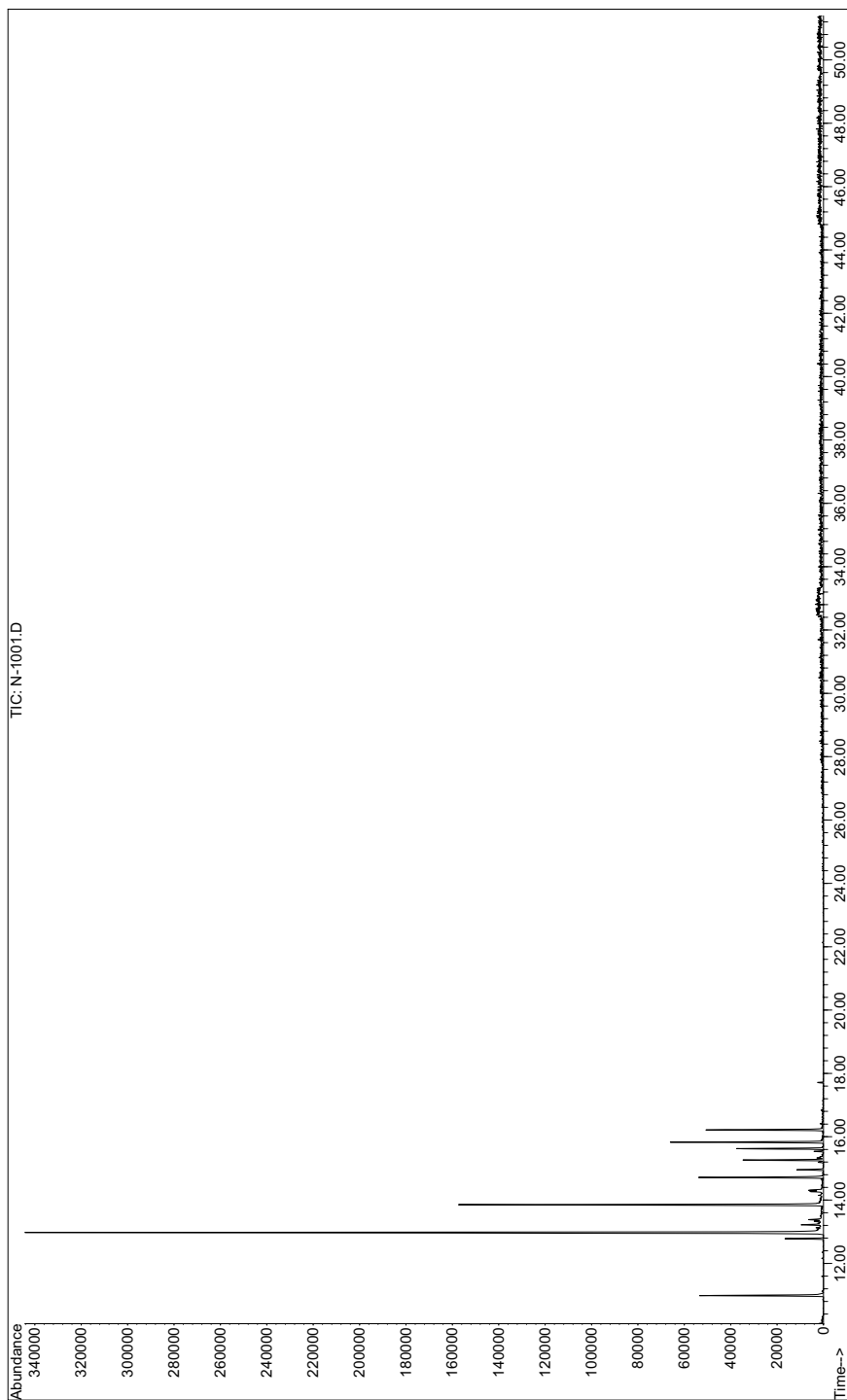
Chromatogram for *Aroclor*[®] 1260 - C-260

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD



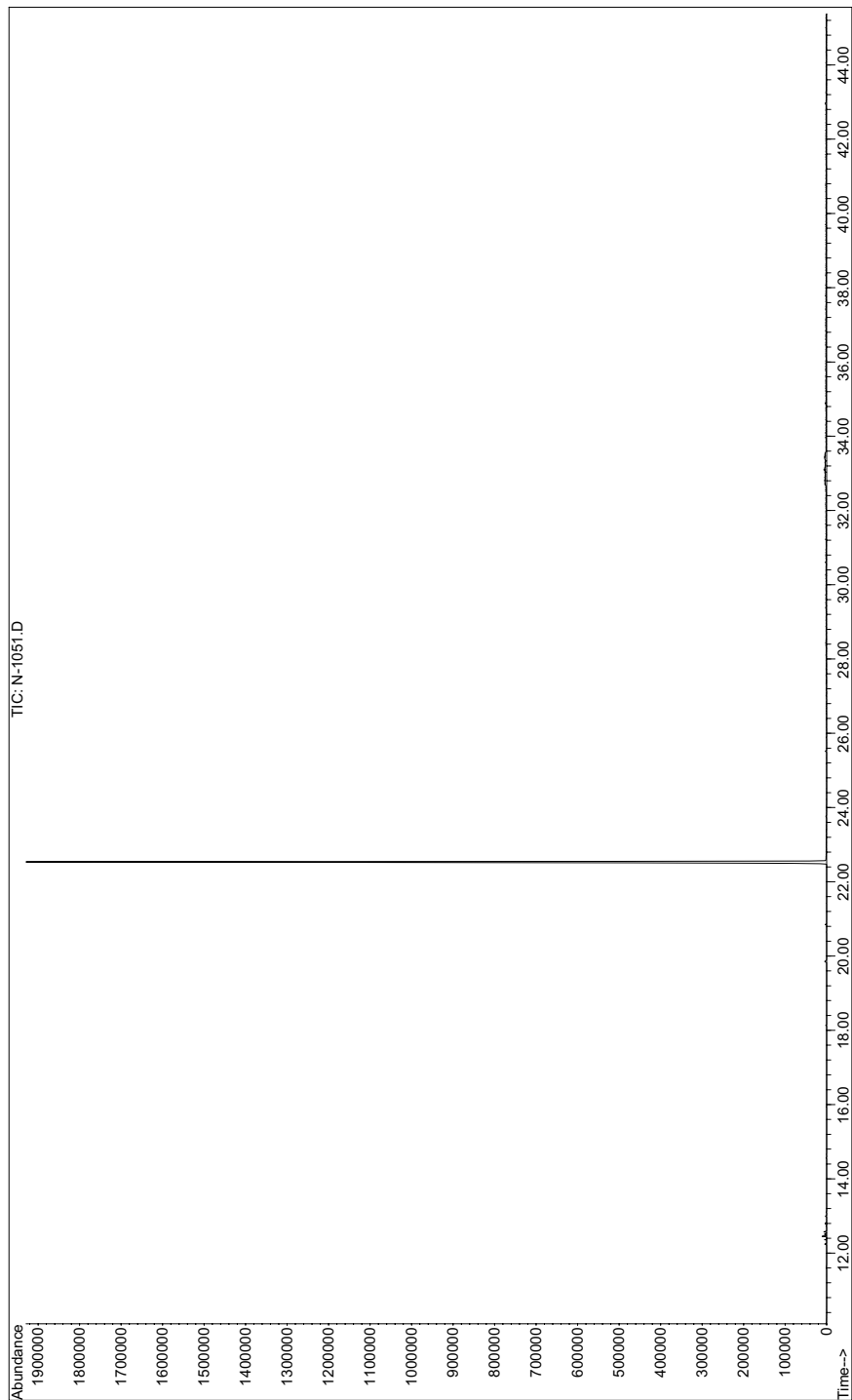
*Analytical Information***Chromatogram for Firemaster BP4A - FRS-006****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

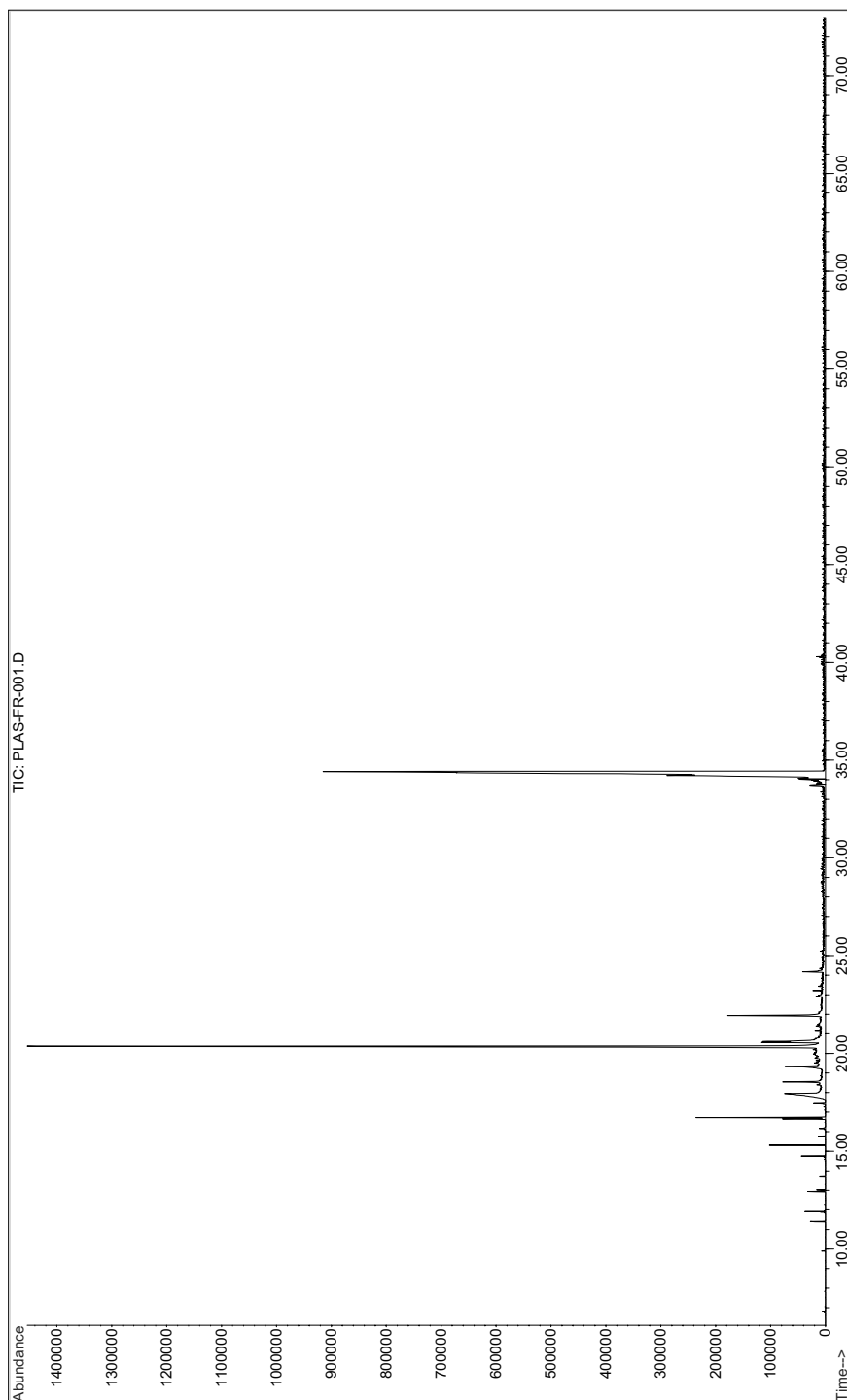
*Analytical Information***Chromatogram for *Halowax 1001 - N-1001*****Analytical Conditions Summary** 80 °C (0 min) to 340 °C (20 min) @ 10 °C/min Det=MSD

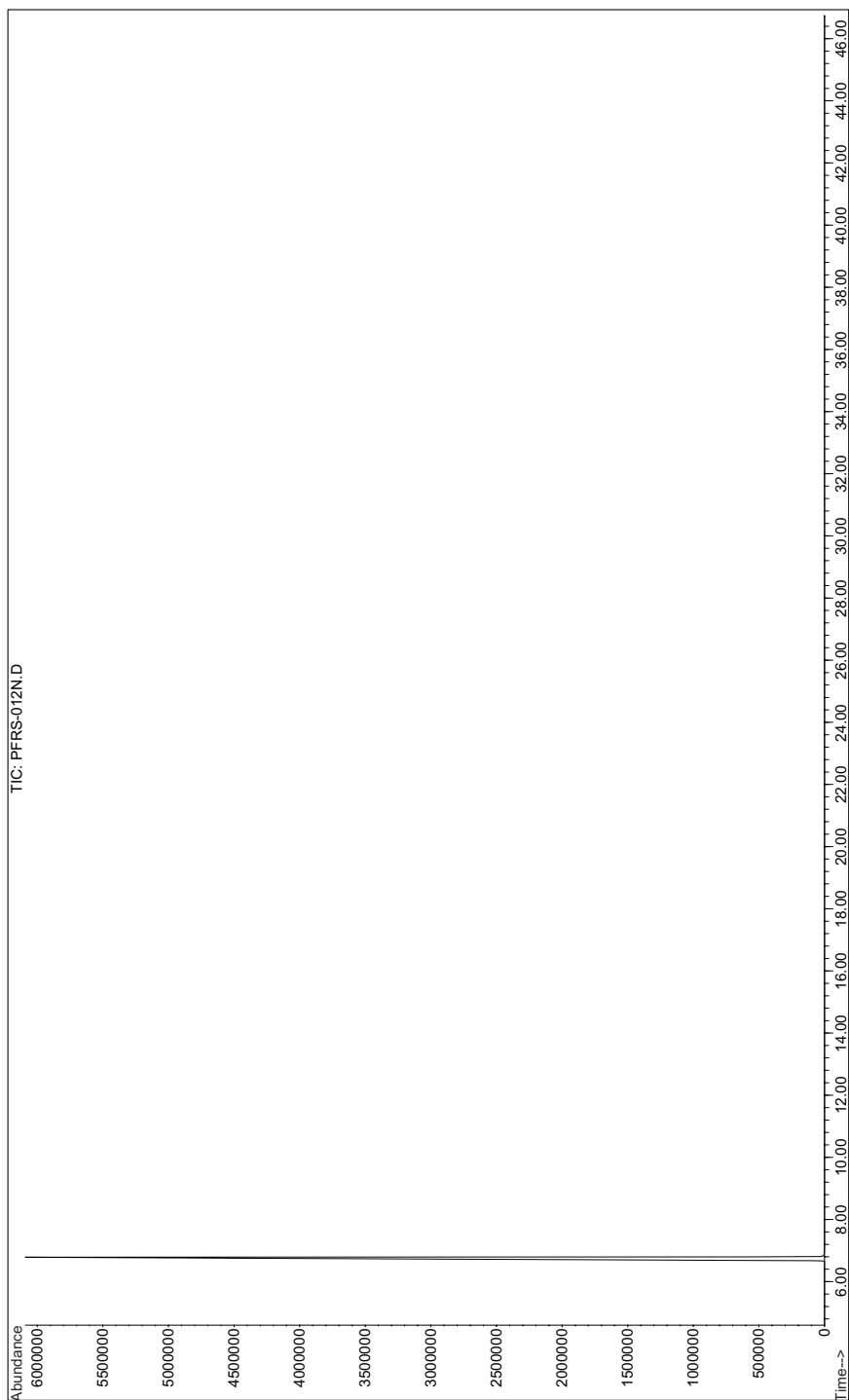
Analytical Information

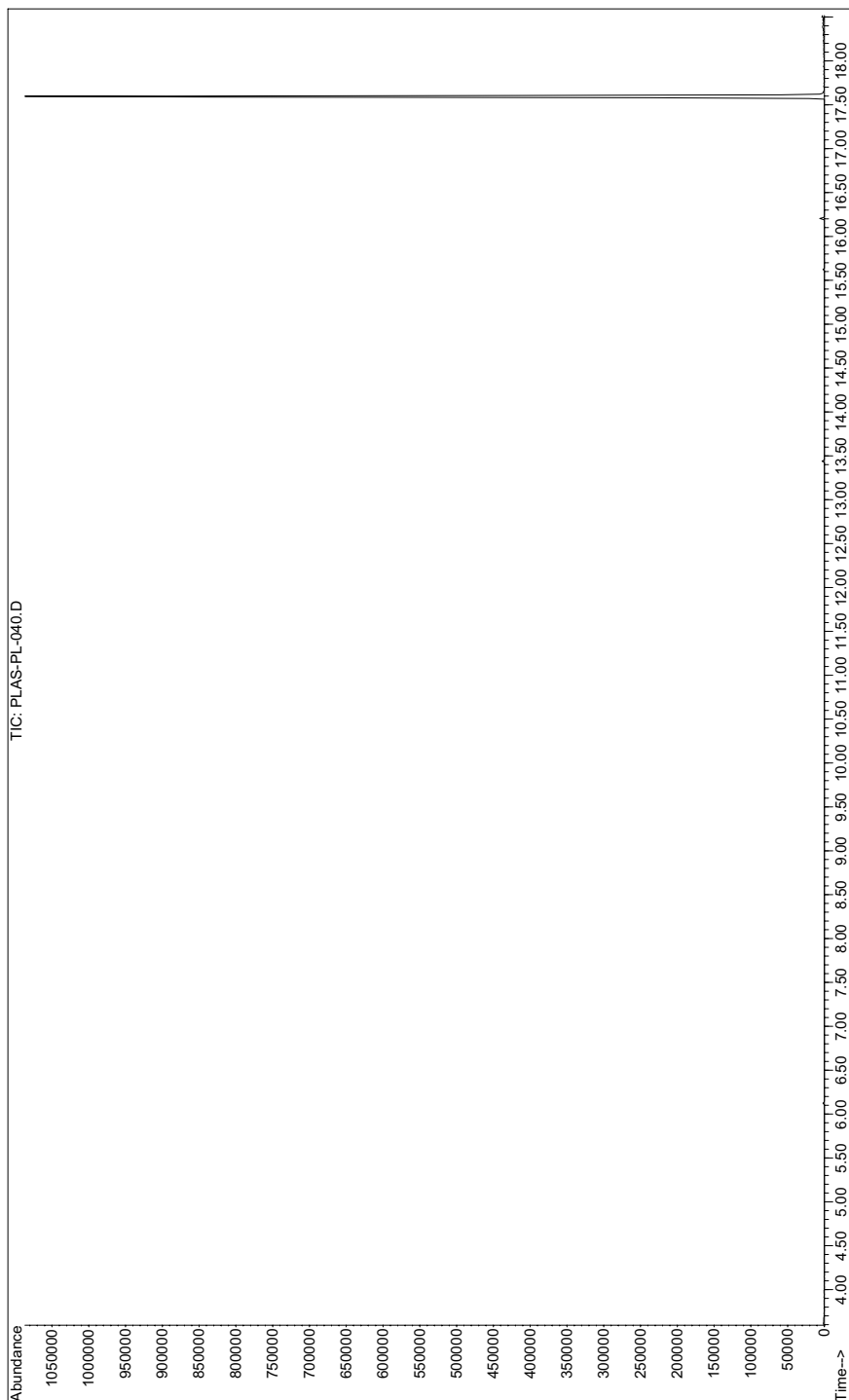
Chromatogram for *Halowax 1051 - N-1051*

Analytical Conditions Summary 80 °C (0 min) to 340 °C (20 min) @ 10 °C/min Det=MSD



*Analytical Information***Chromatogram for Saytex[®] 8010 - PLAS-FR-001****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

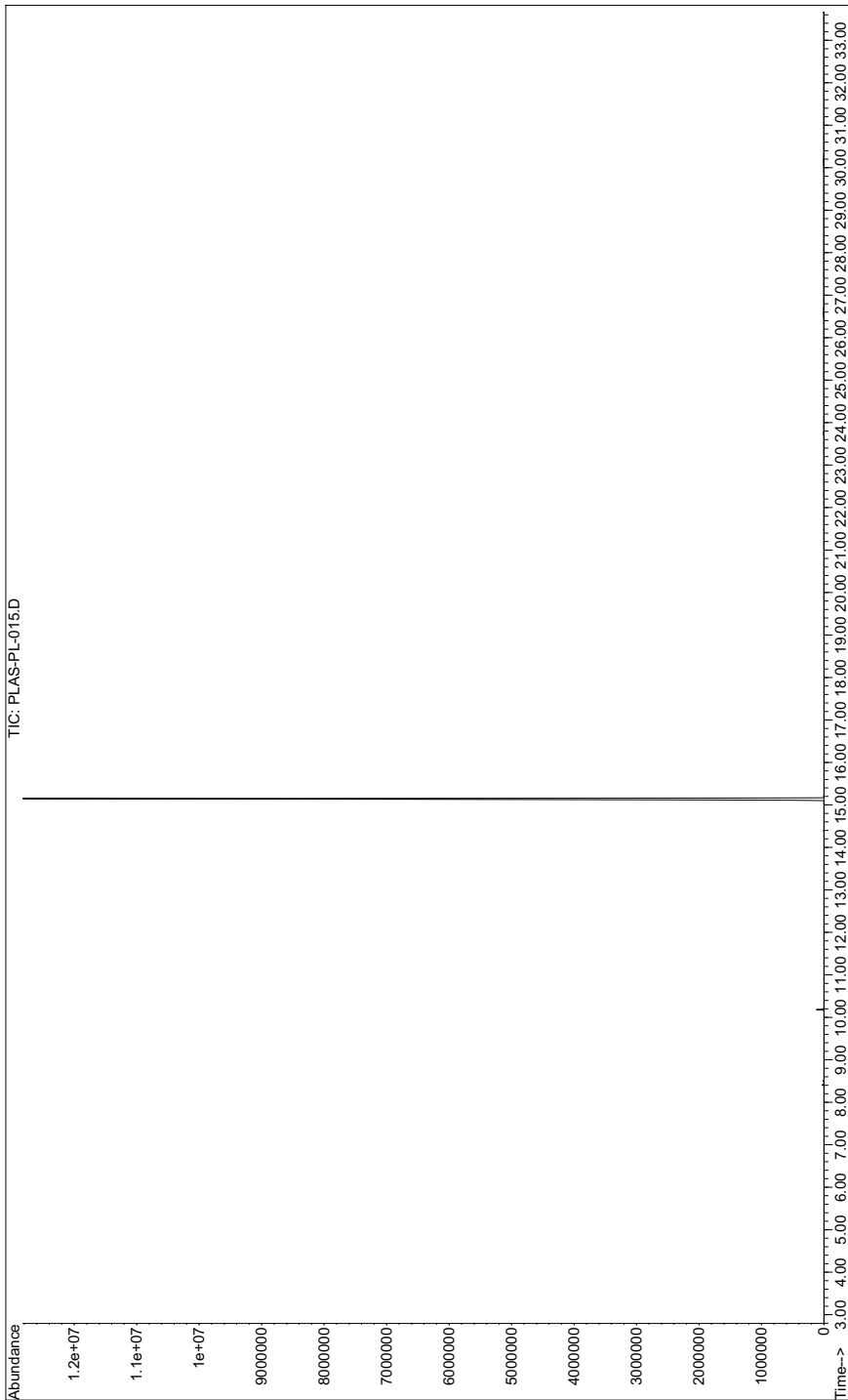
*Analytical Information***Chromatogram for Triethylphosphate - PFRS-012****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

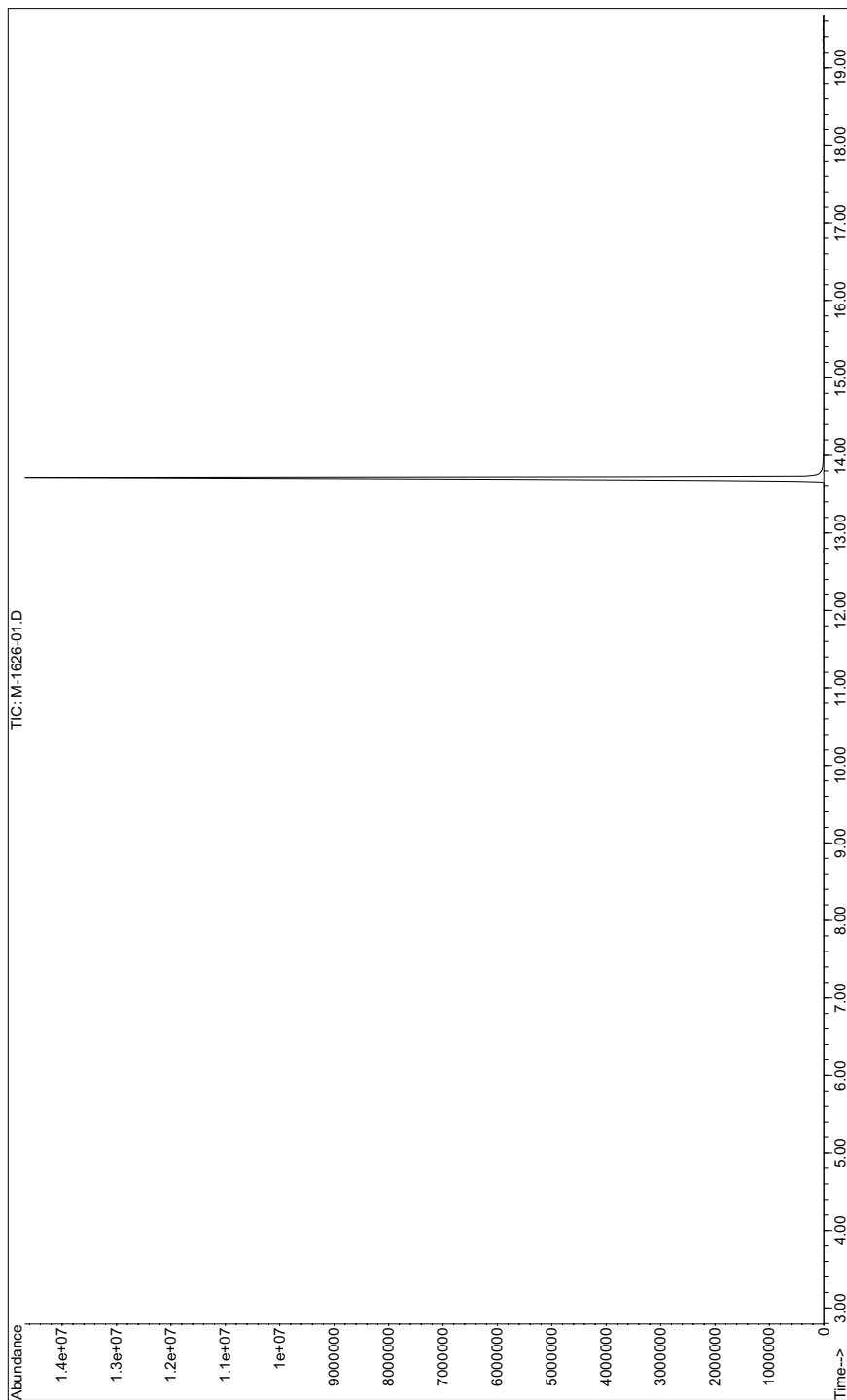
*Analytical Information***Chromatogram for *Adimoll DO - PLAS-PL-040*****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

Analytical Information

Chromatogram for *Benzoflex*® 2-45 - PLAS-PL-015

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

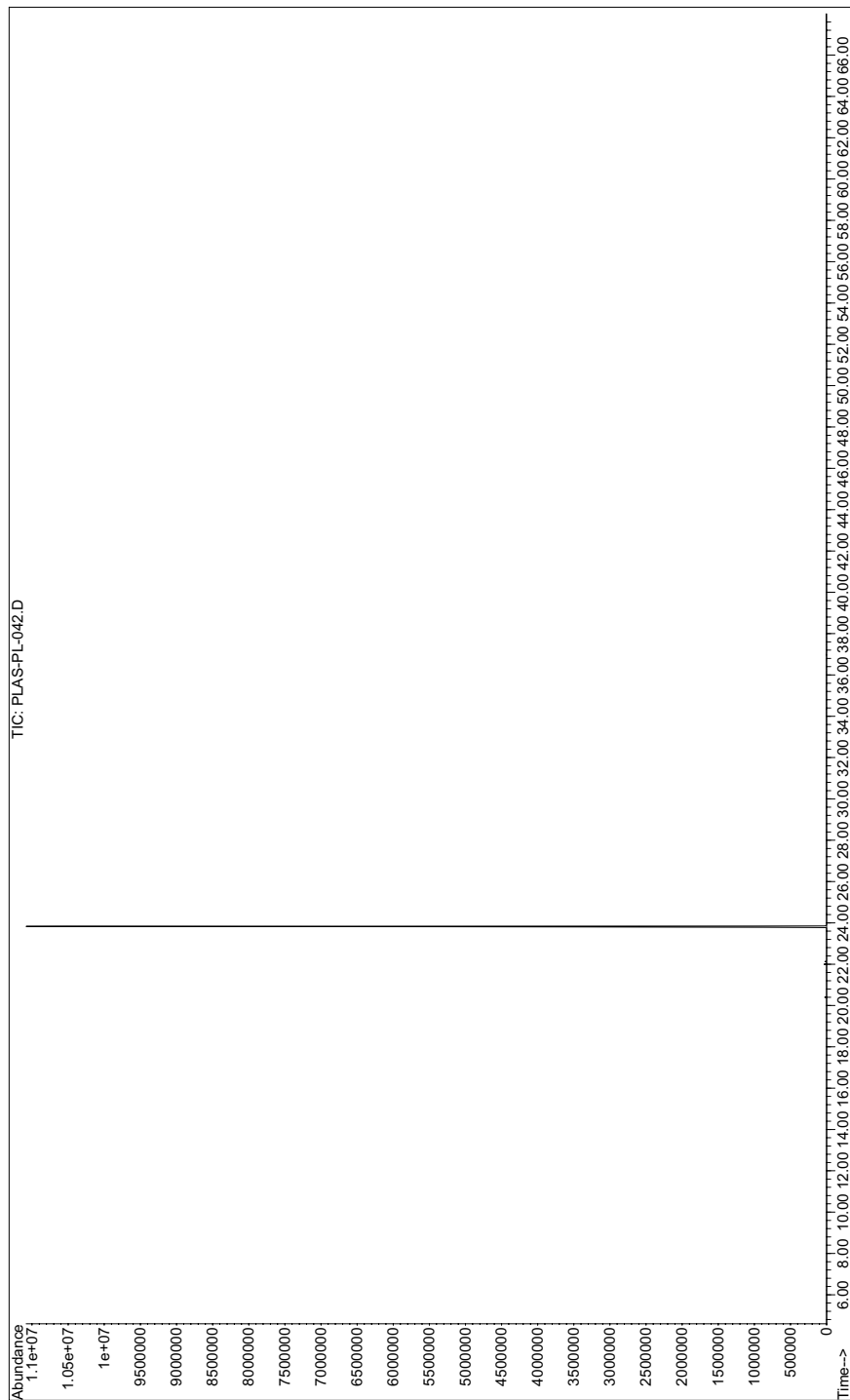


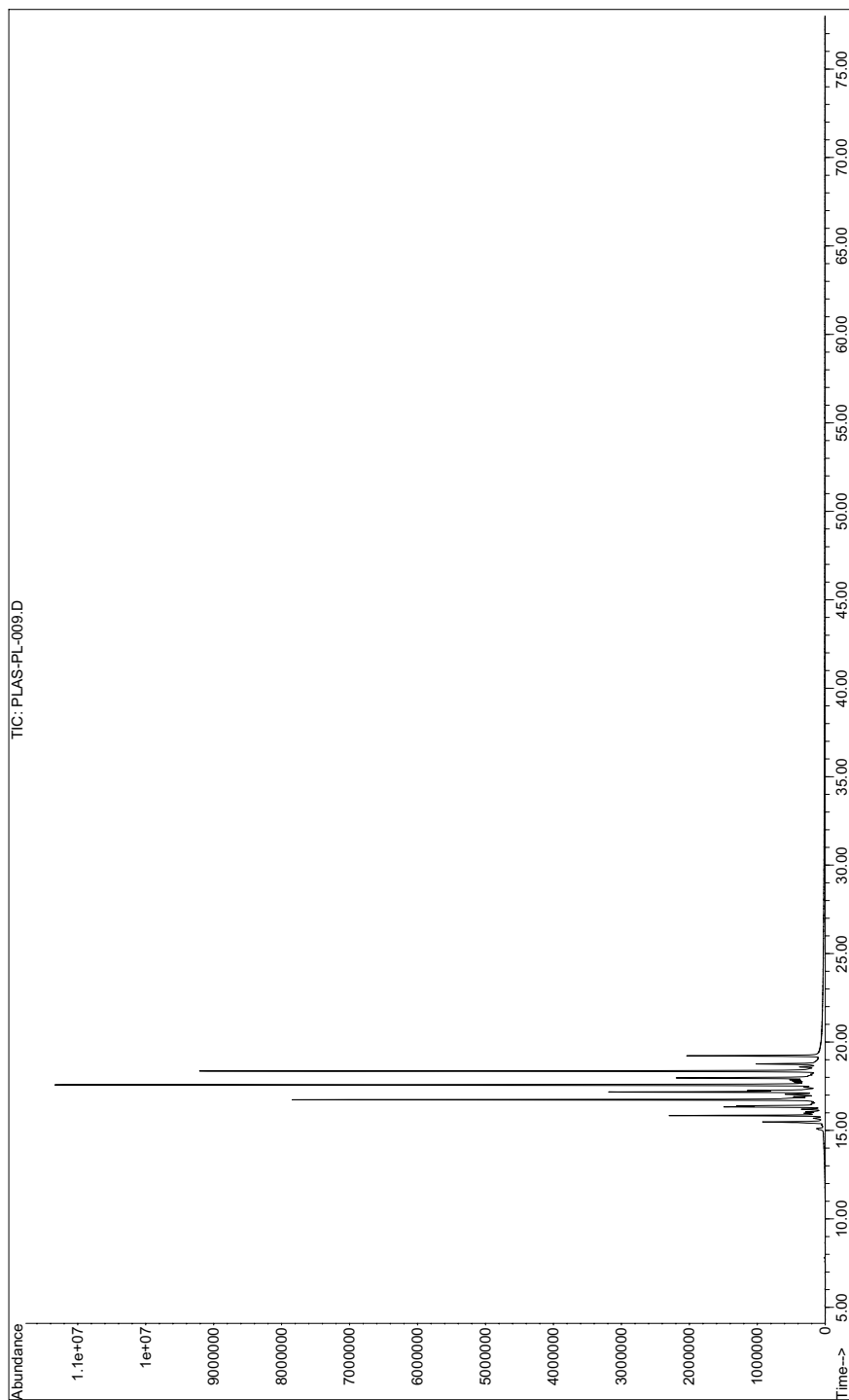
*Analytical Information***Chromatogram for *Bisphenol A* - M-1626-01****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

Analytical Information

Chromatogram for *Butyl ricinoleate* - PLAS-PL-042

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

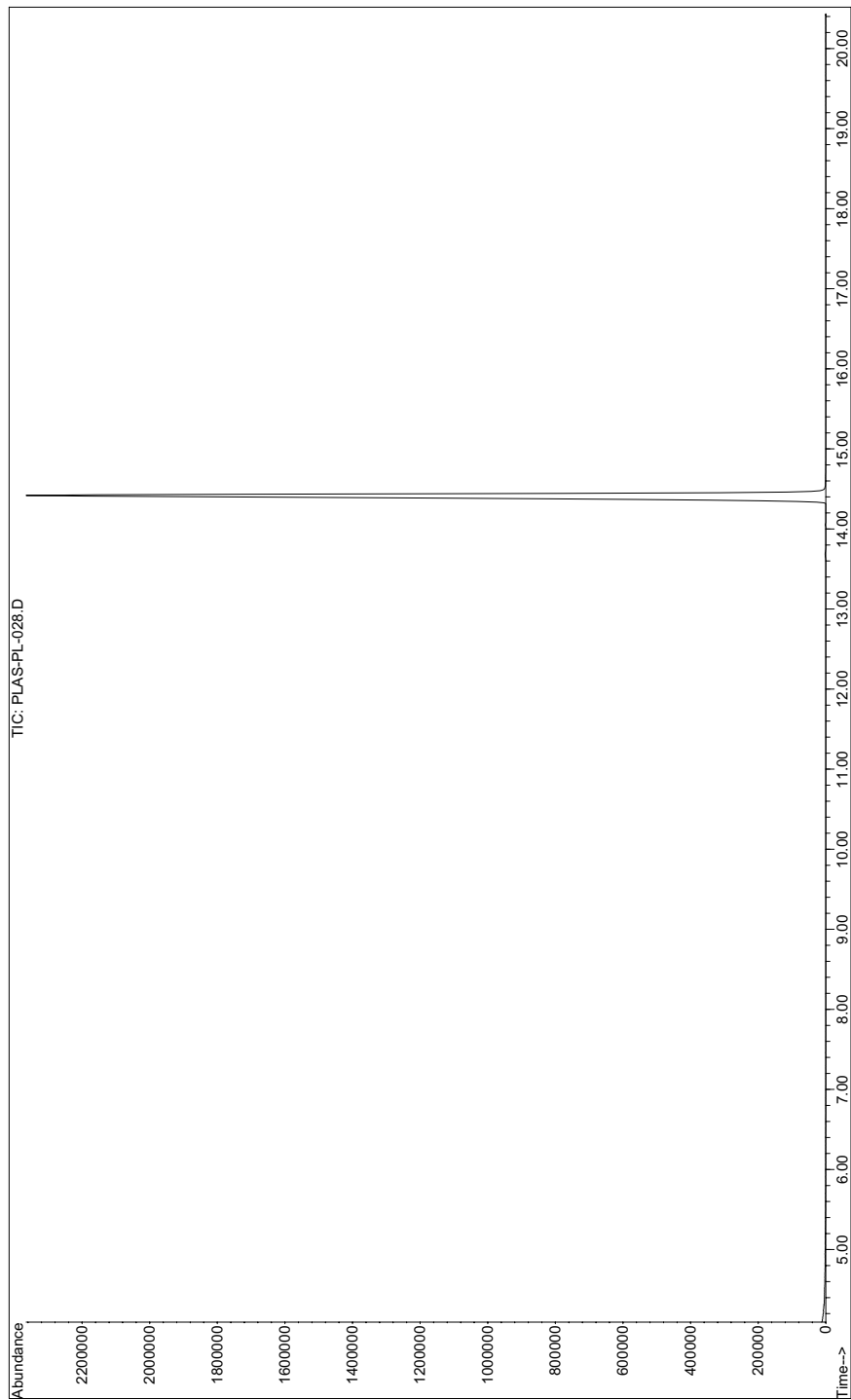


*Analytical Information***Chromatogram for Celogen® SD-I25 - PLAS-PL-009****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD

Analytical Information

Chromatogram for *Citroflex*[®] 2 - PLAS-PL-028

Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/minDet=MSD

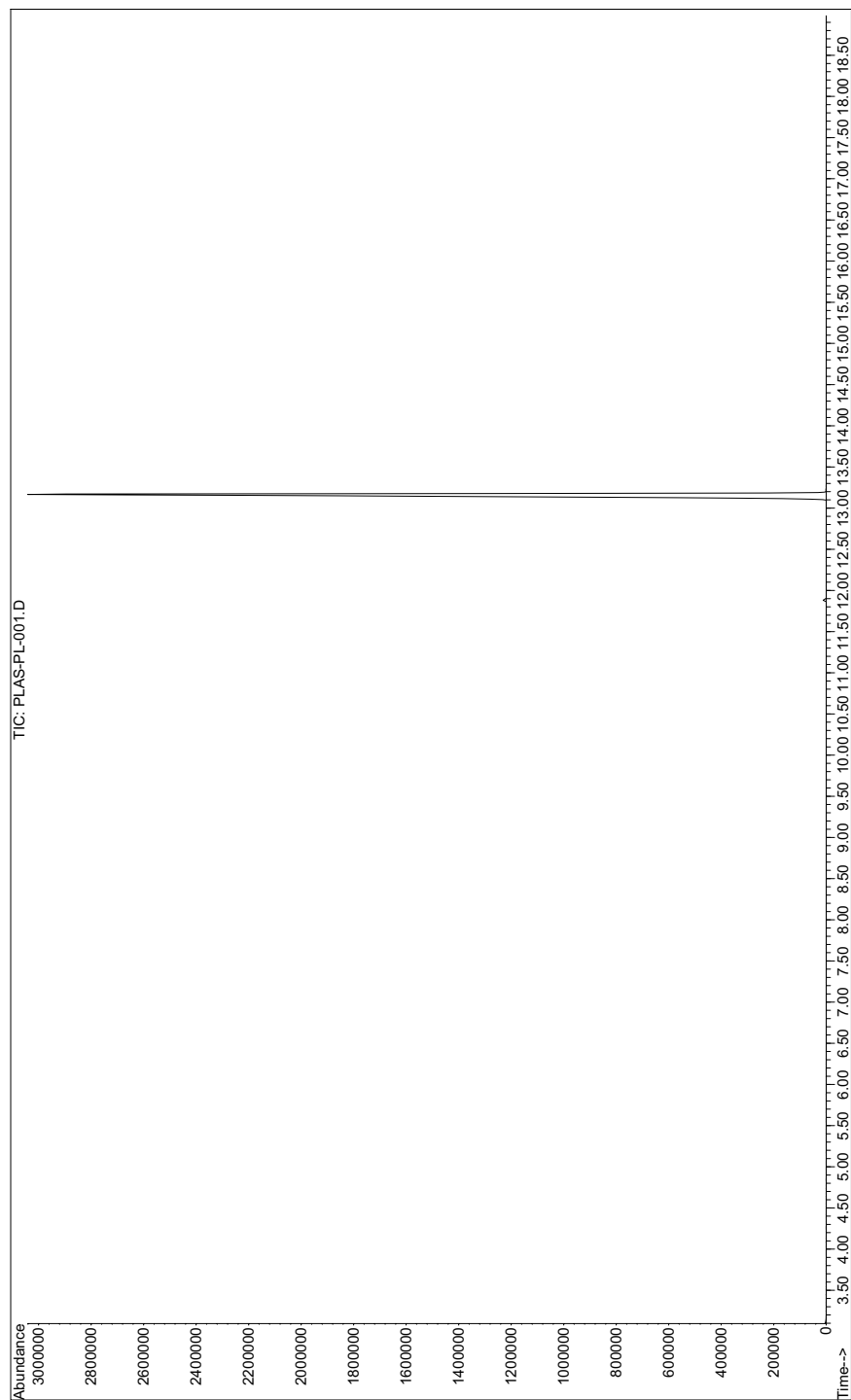


*Analytical Information***Chromatogram for *Citroflex*[®] 4 - PLAS-PL-030****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

Analytical Information

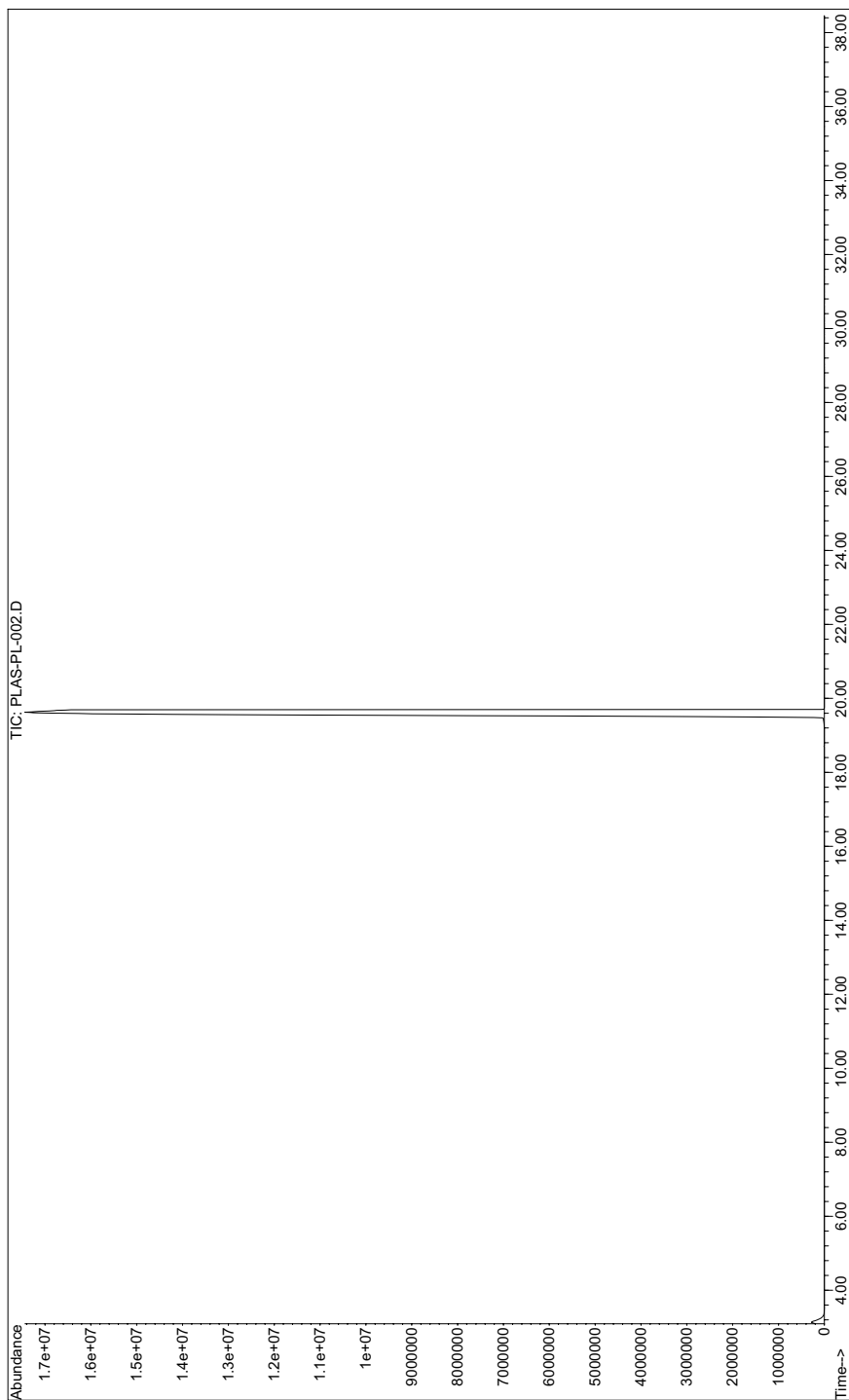
Chromatogram for *Citroflex*[®] A-2 - PLAS-PL-001

Analytical Conditions Summary 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD



*Analytical Information***Chromatogram for *Citroflex*[®] A-4 - PLAS-PL-002****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

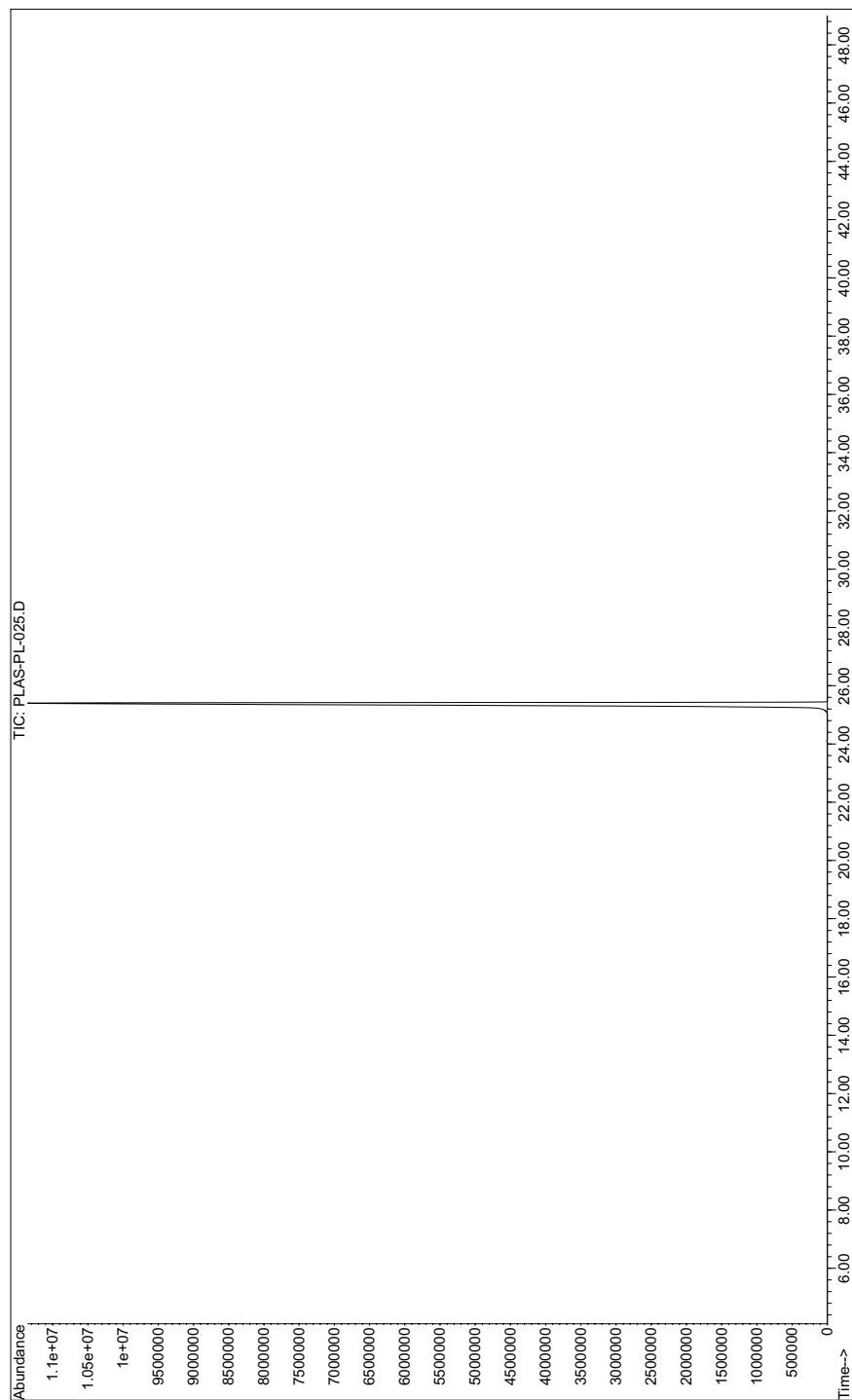
Inj Temp=250 °C, Det=MSD

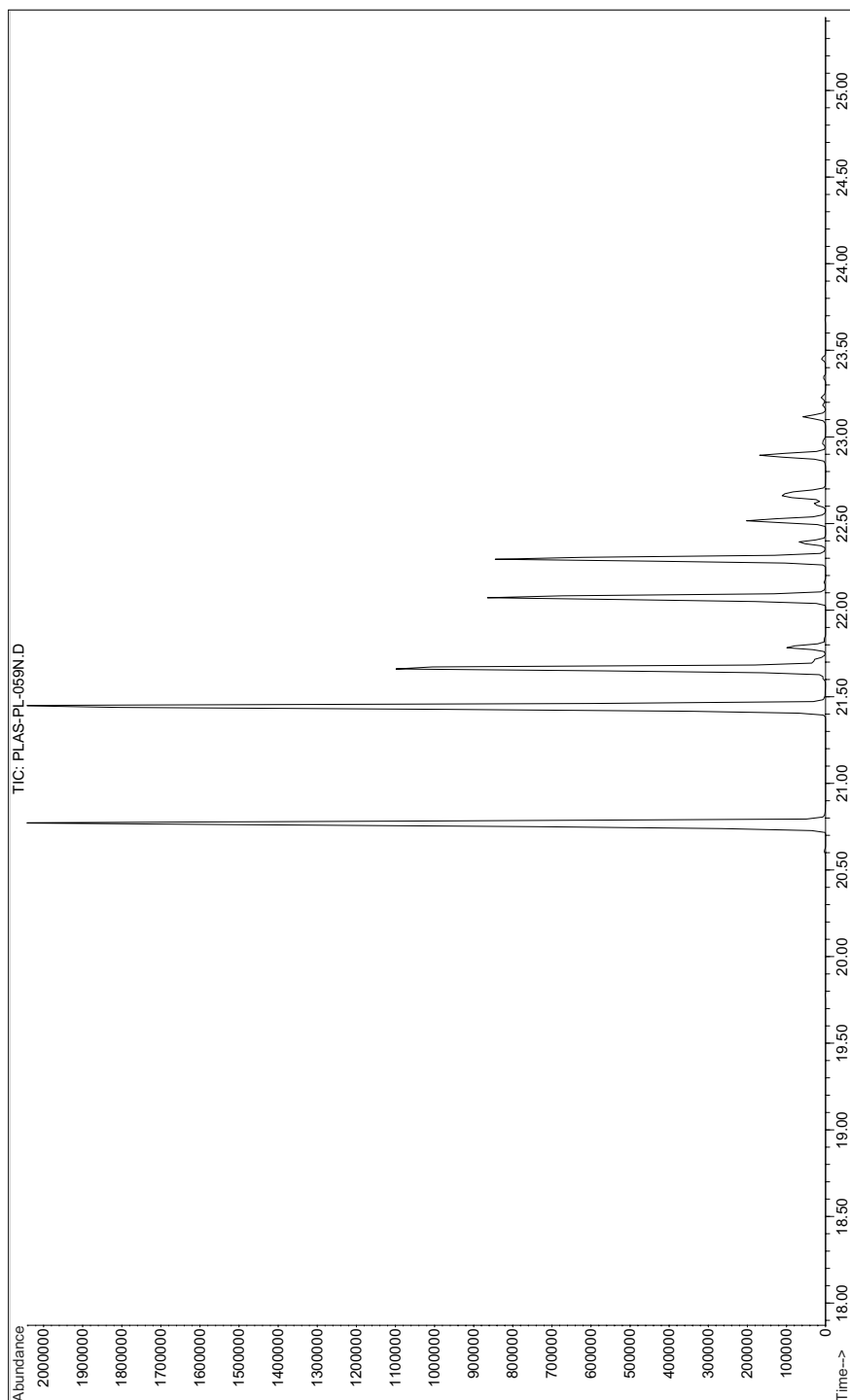


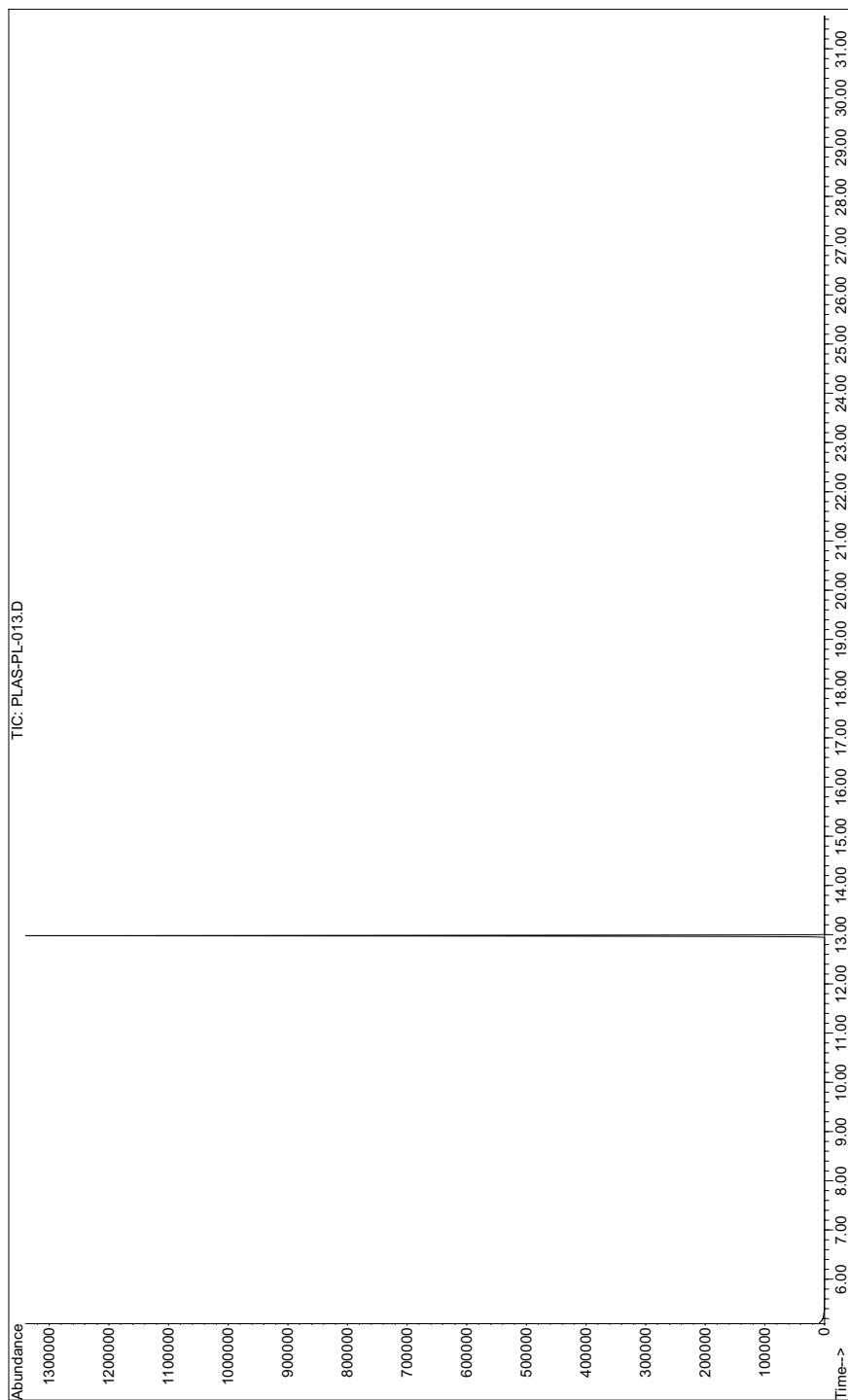
Analytical Information

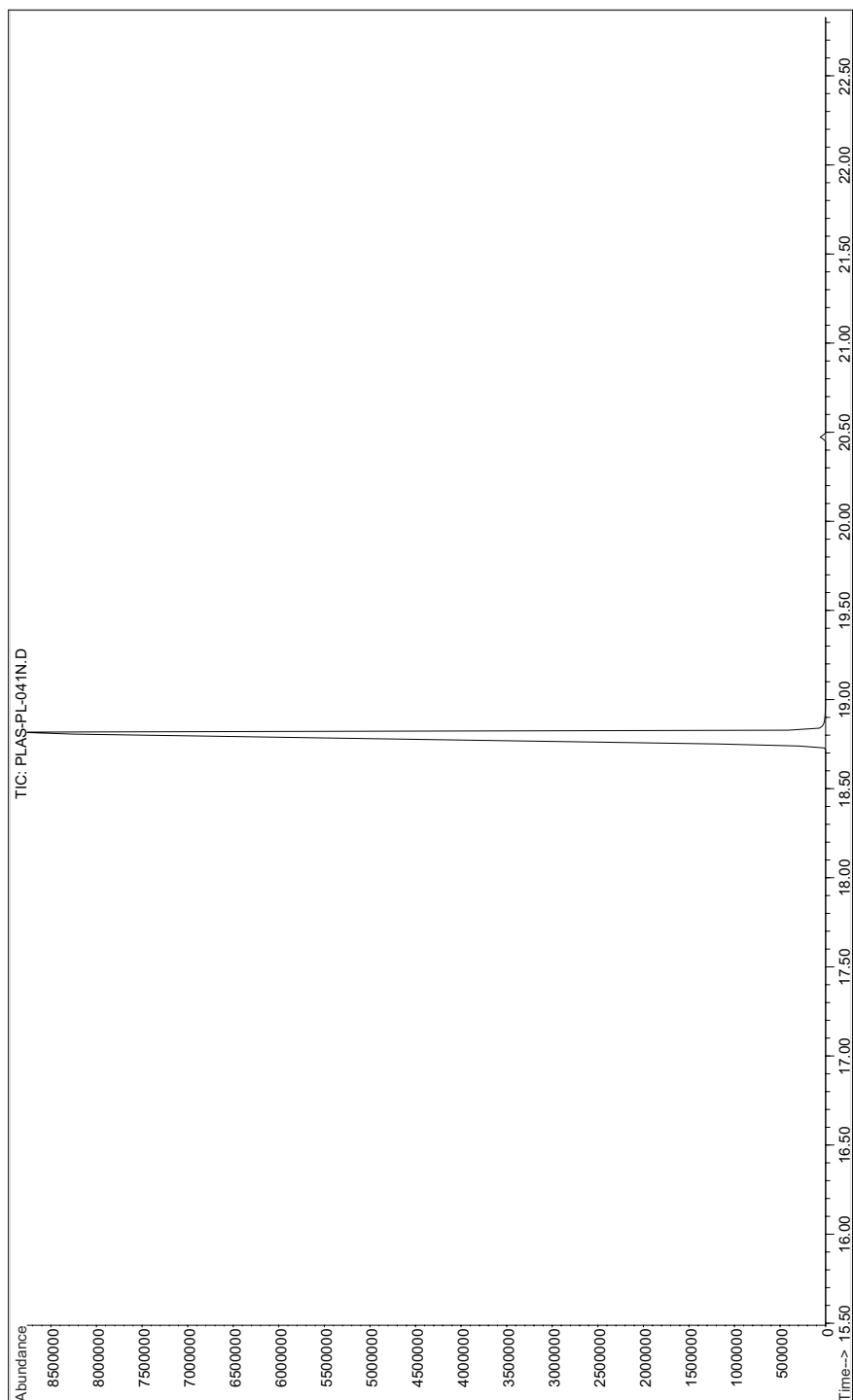
Chromatogram for *Citroflex*[®] B-6 - PLAS-PL-025

Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



*Analytical Information***Chromatogram for *Cresyl Diphenyl Phosphate - PLAS-PL-059*****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

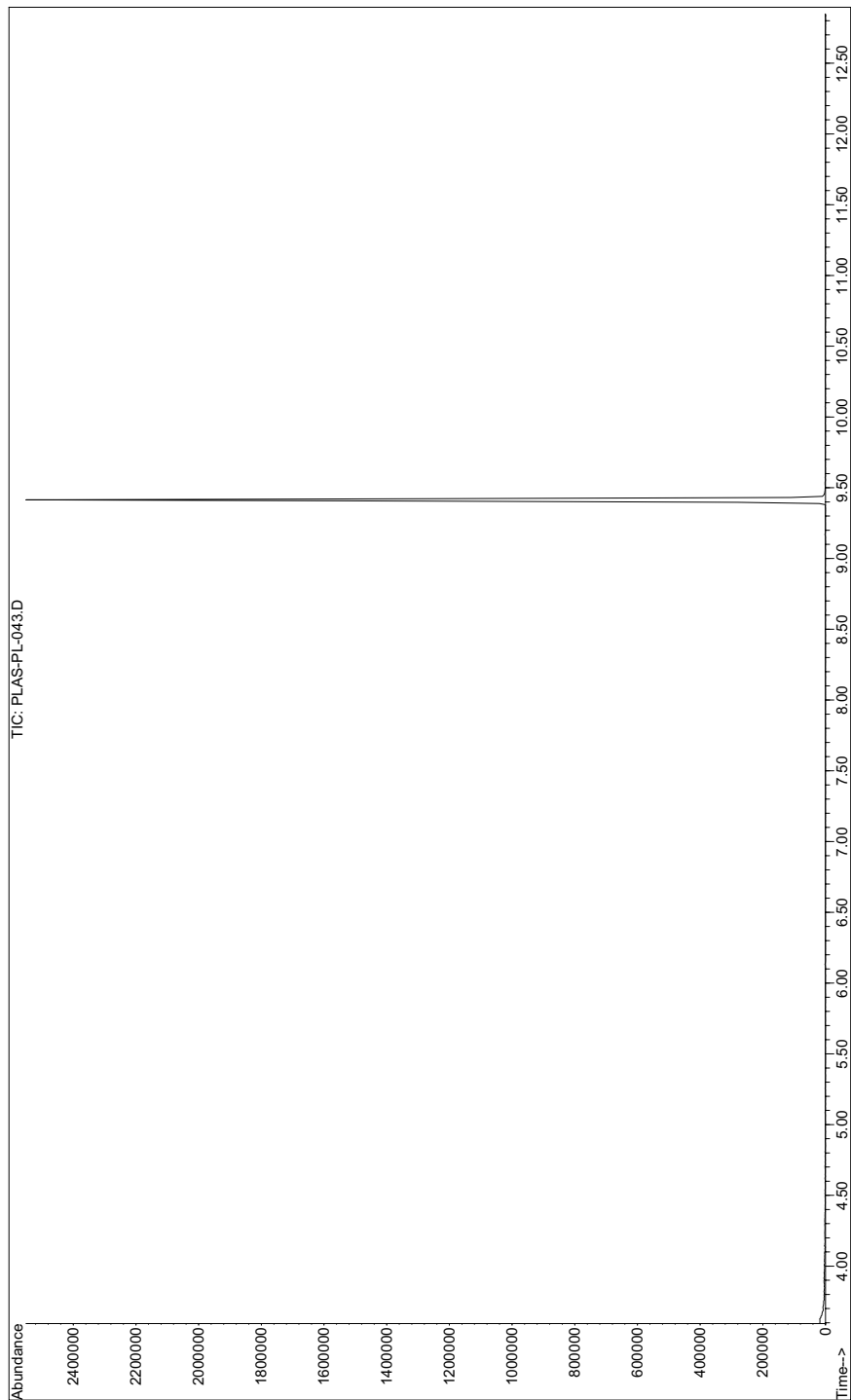
*Analytical Information***Chromatogram for *Dibutyl Phthalate* - PLAS-PL-013****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

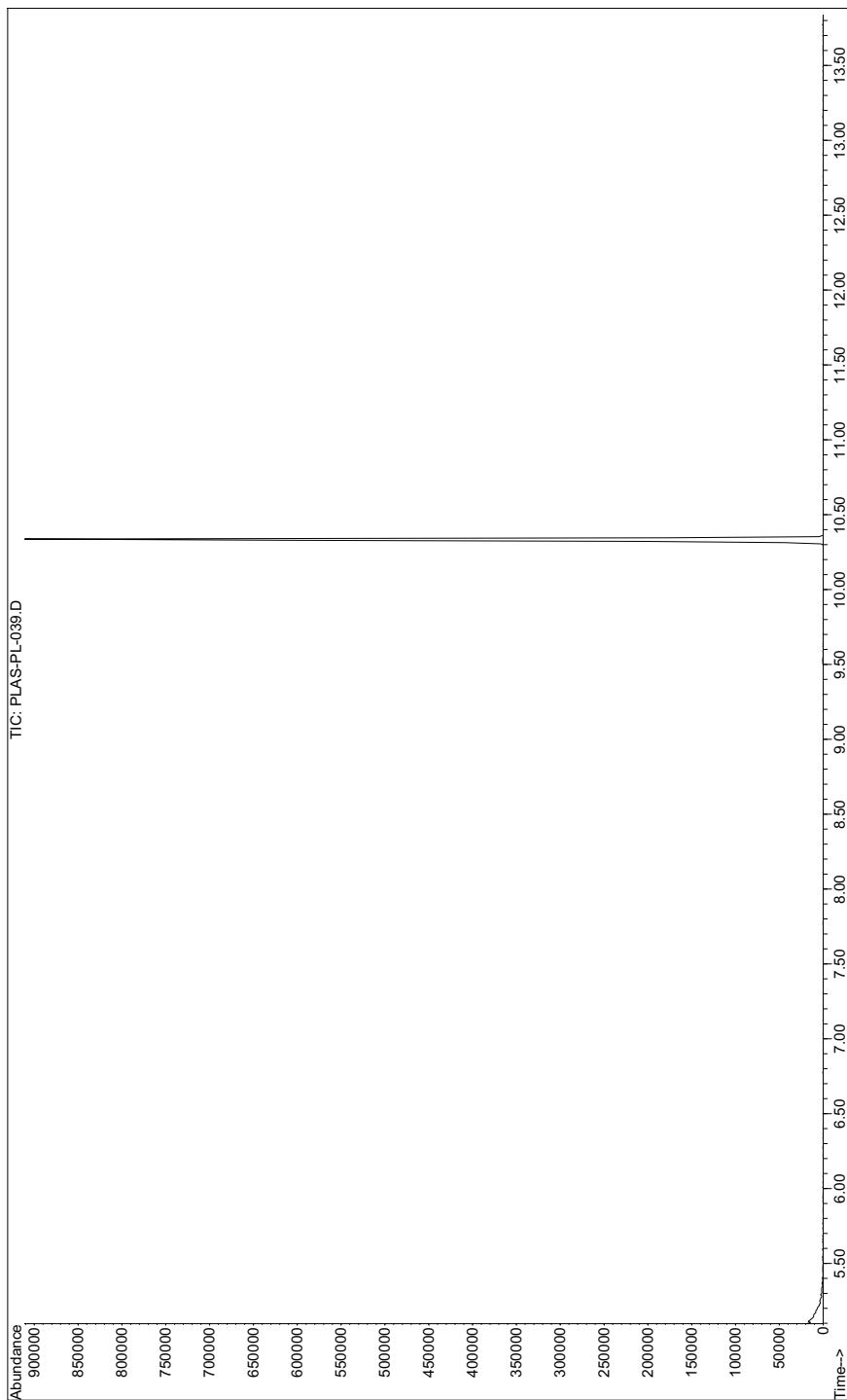
*Analytical Information***Chromatogram for *Dibutyl Sebacate* - PLAS-PL-041****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for*Diethyl adipate - PLAS-PL-043*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

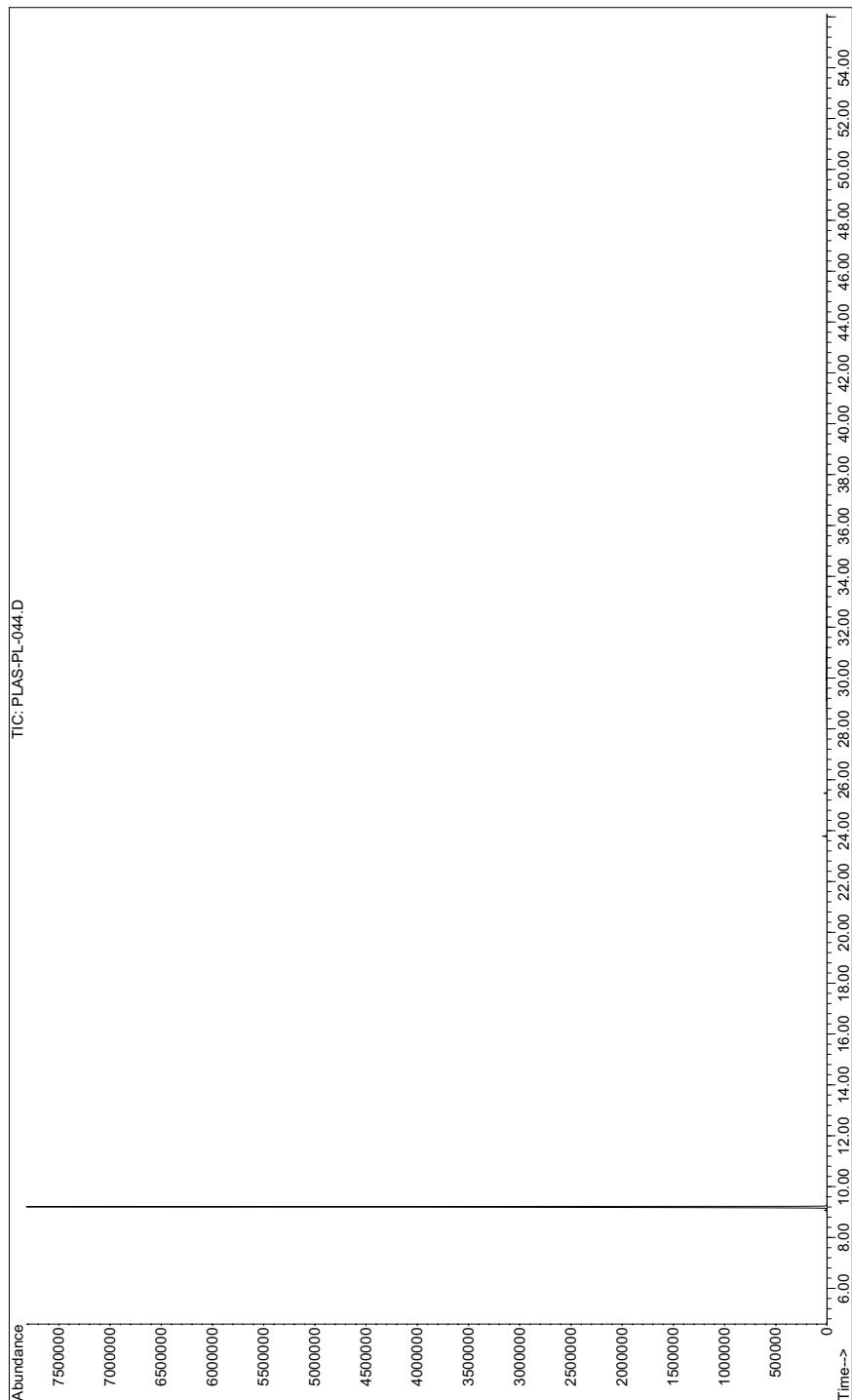


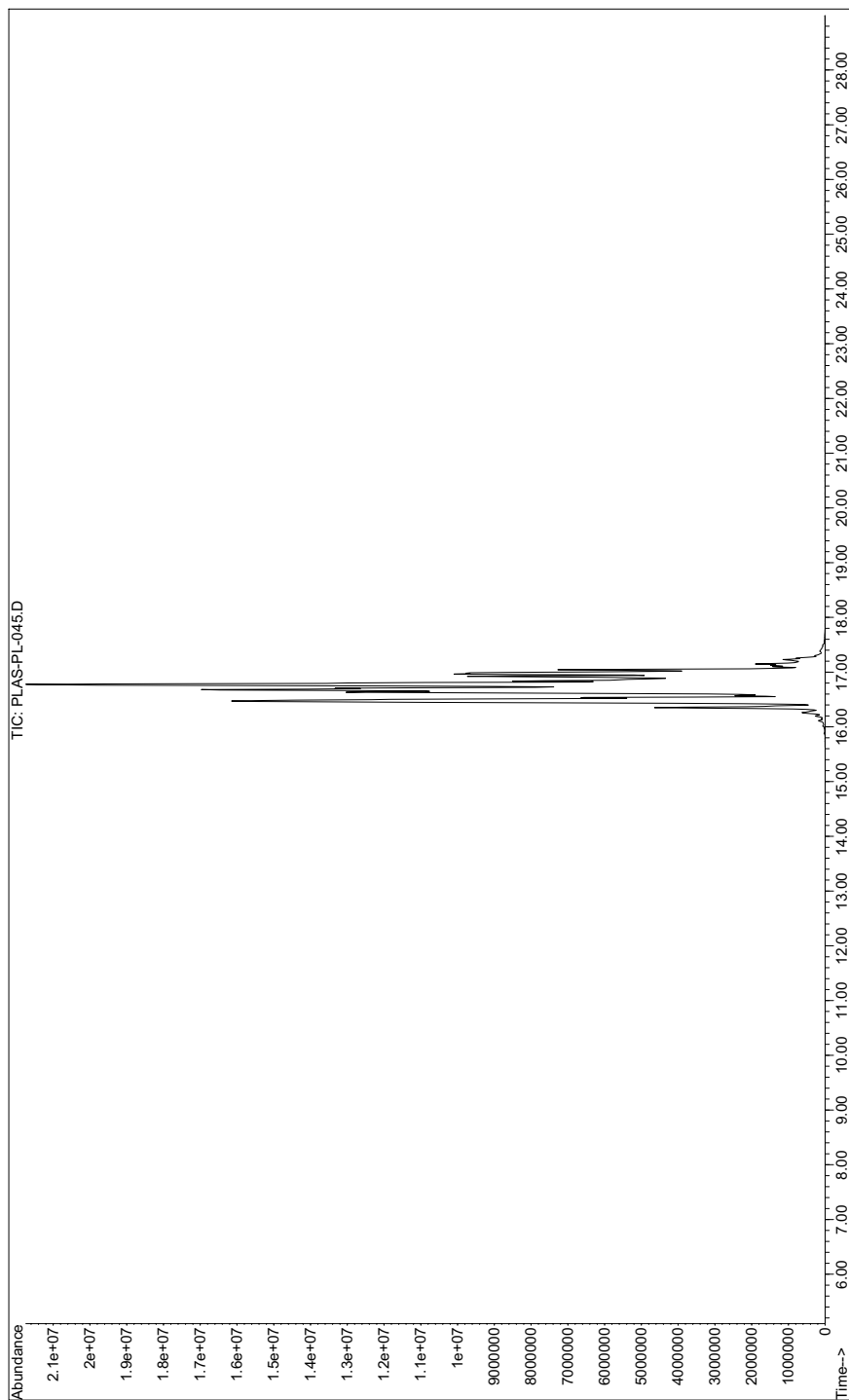
*Analytical Information***Chromatogram for *Diethyl phthalate* - PLAS-PL-039****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

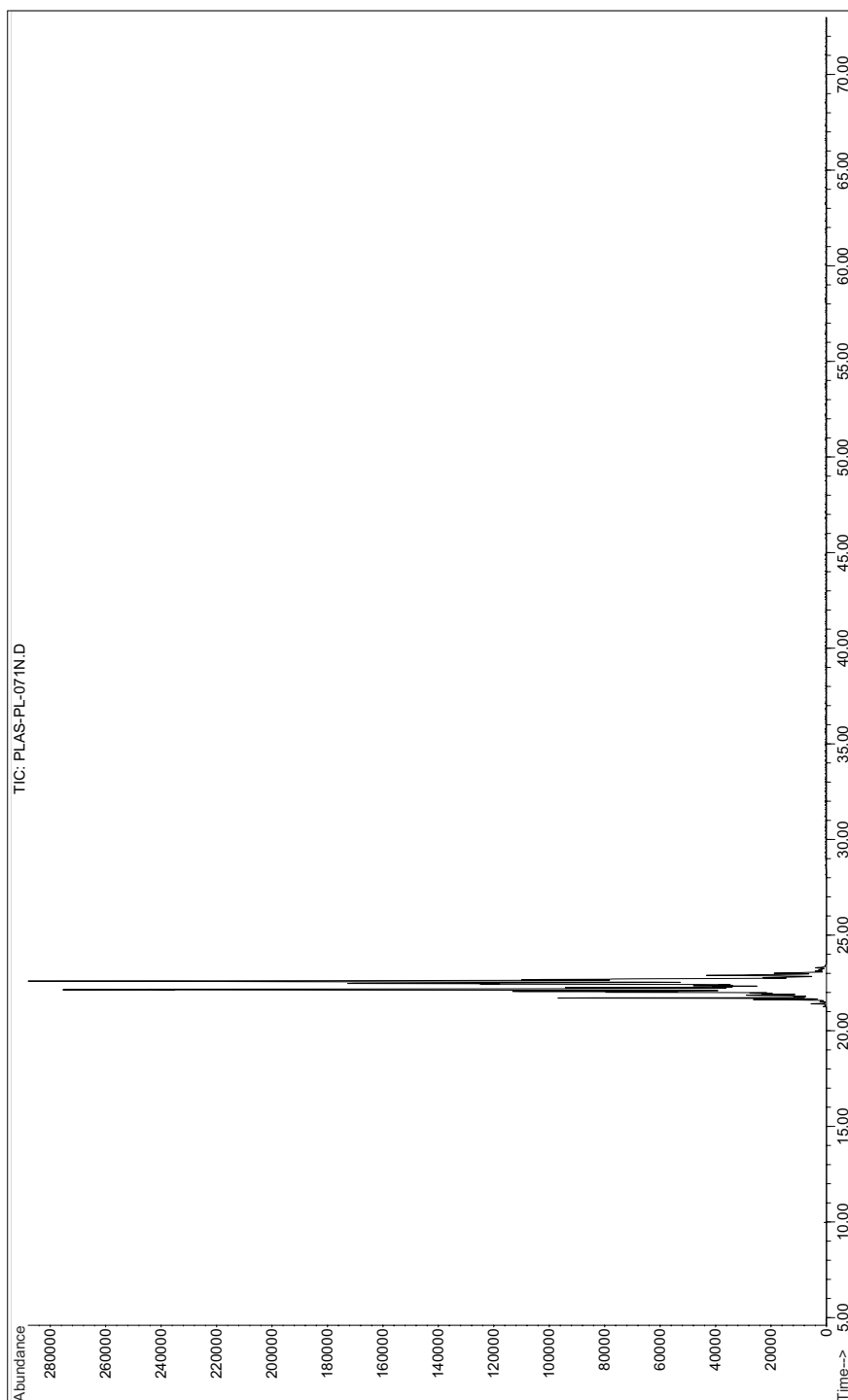
Analytical Information

Chromatogram for *Diethyl succinate* - PLAS-PL-044

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



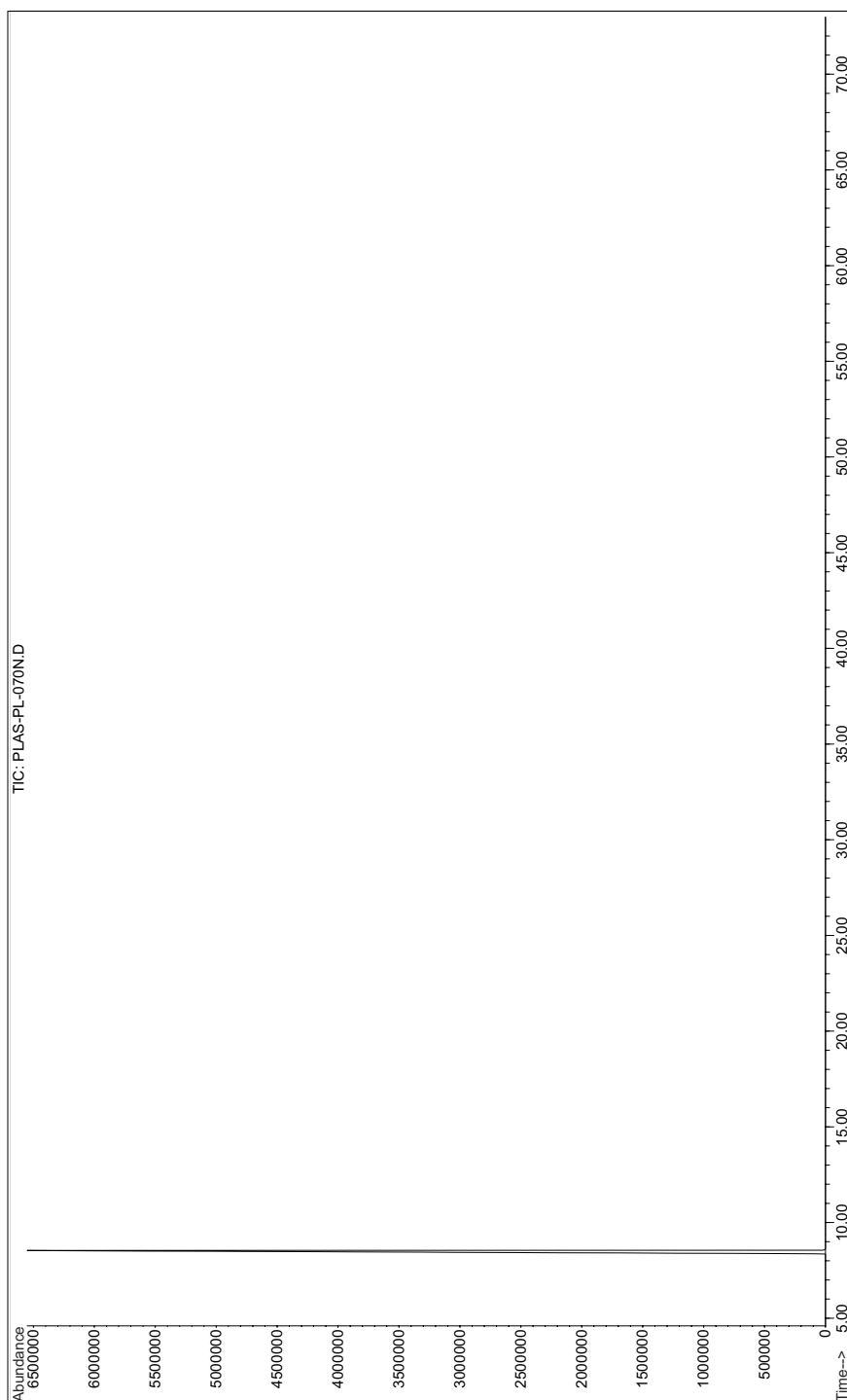
*Analytical Information***Chromatogram for *Diisononyl adipate* - PLAS-PL-045****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

*Analytical Information***Chromatogram for *Diisooctyl phthalate* - PLAS-PL-071****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *Dimethyl adipate - PLAS-PL-070*

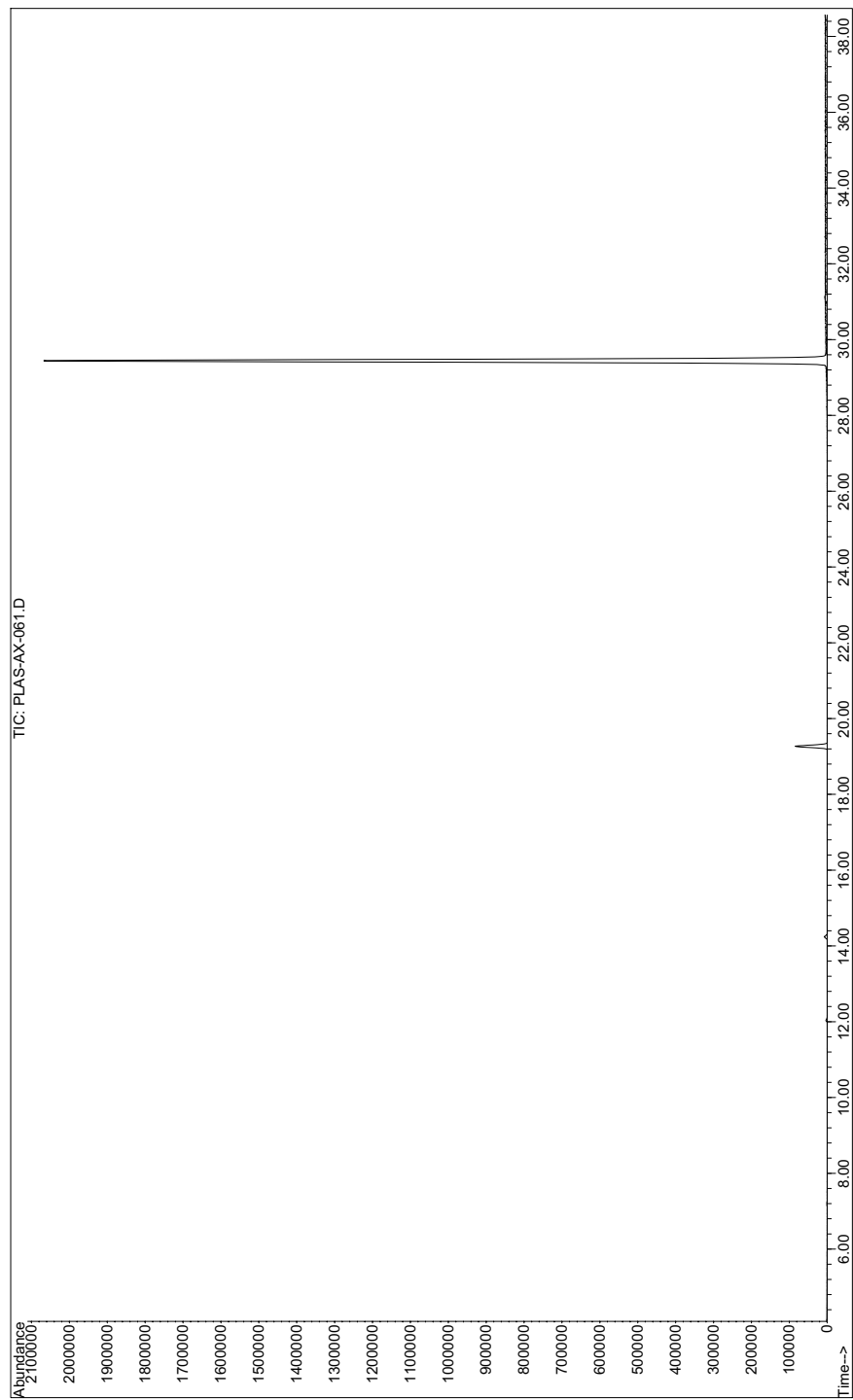
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

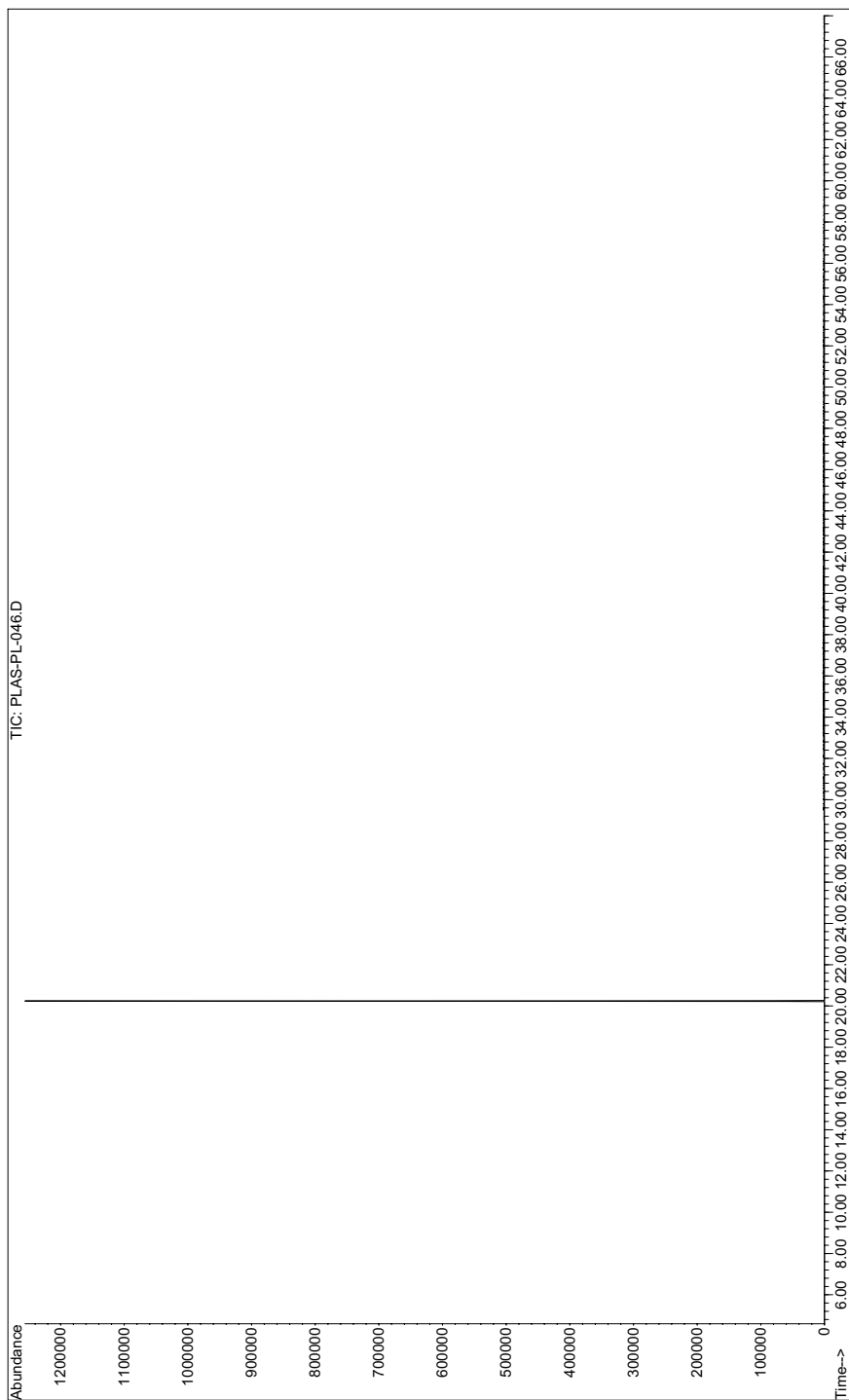
Chromatogram for *Dimethyl Sebacate* - PLAS-PL-061

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *Diocetyl maleate* - PLAS-PL-046****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

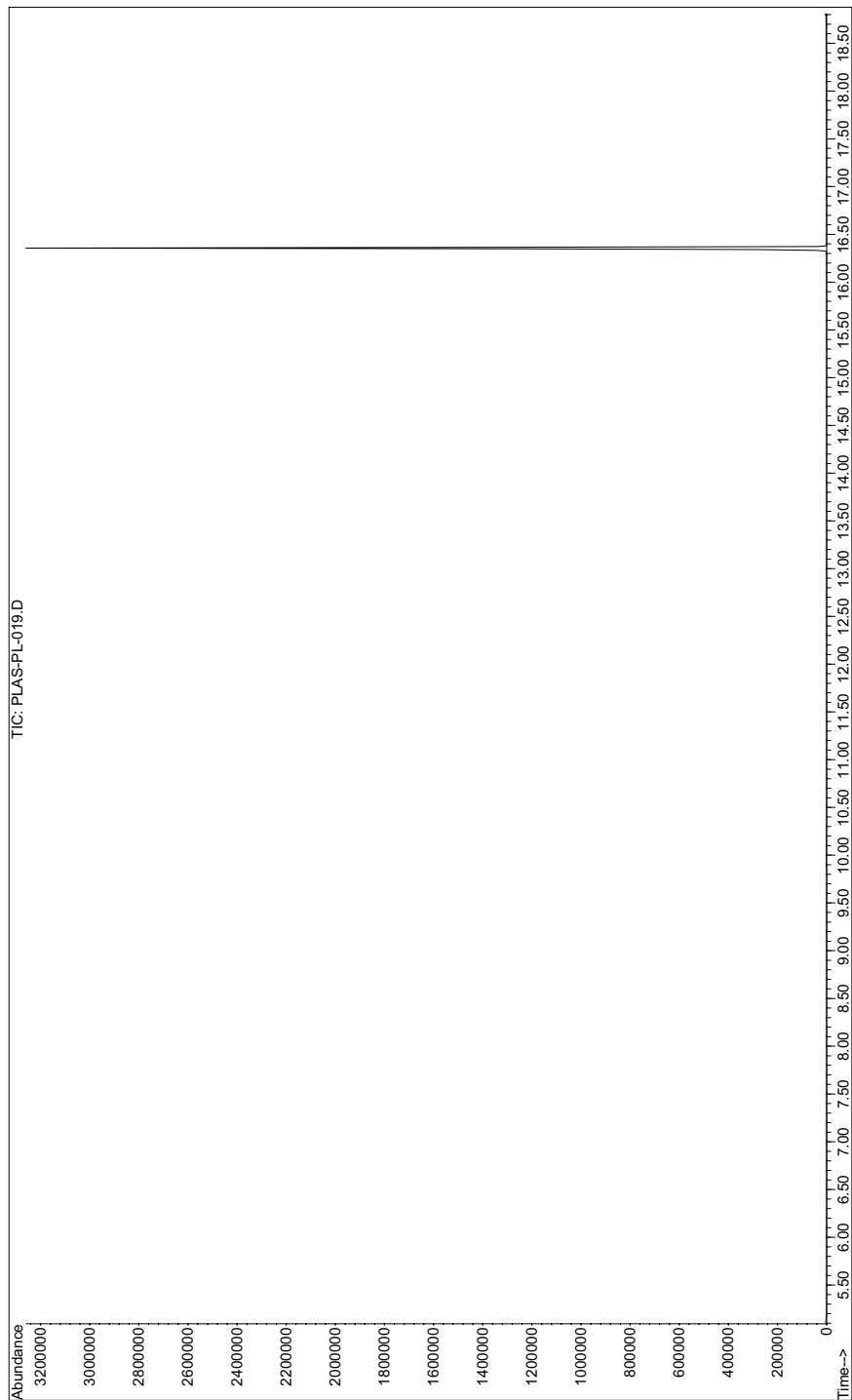
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Diethyl phthalate (DOP)* - PLAS-PL-019

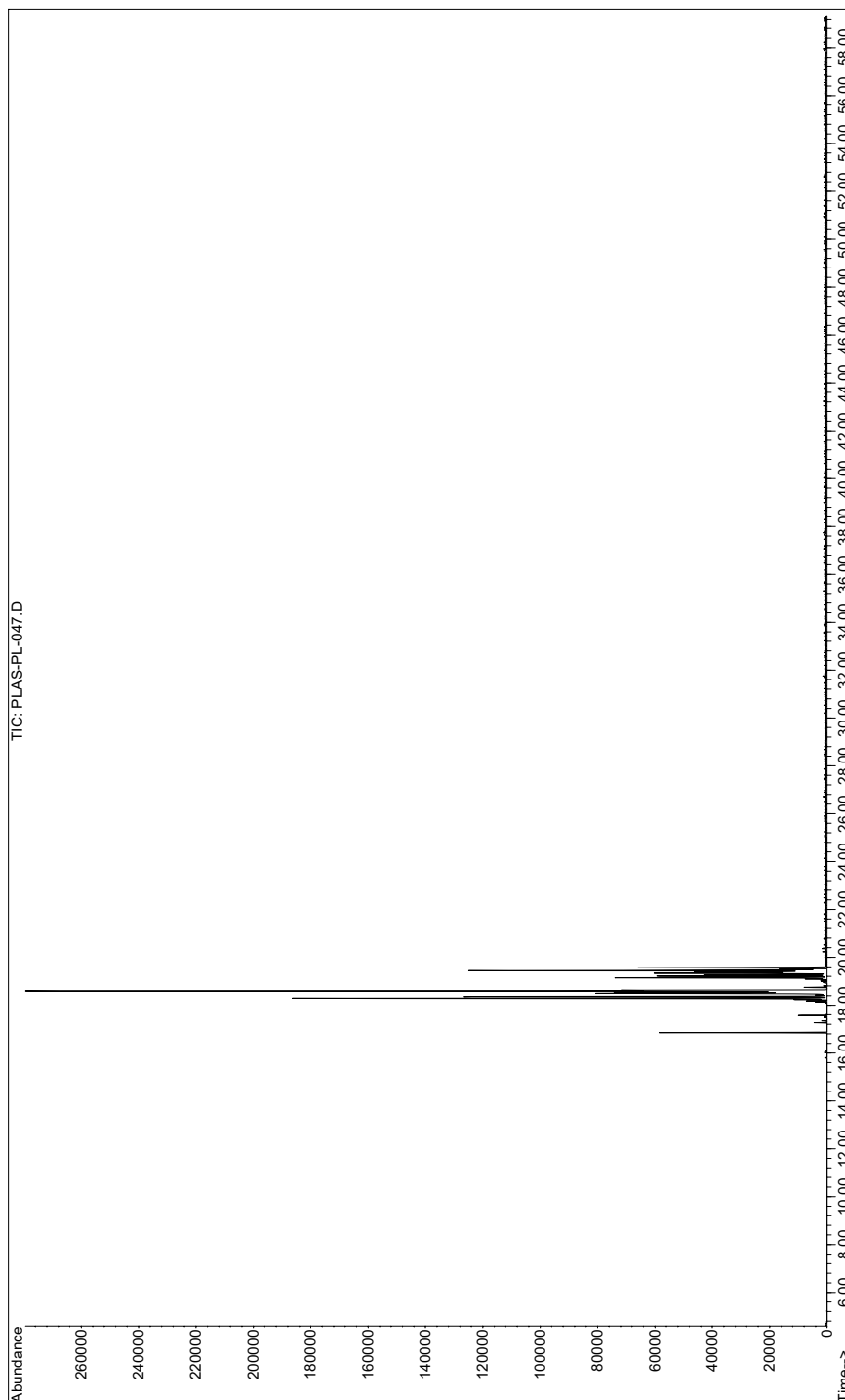
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Epoxidized linseed oil - PLAS-PL-047*

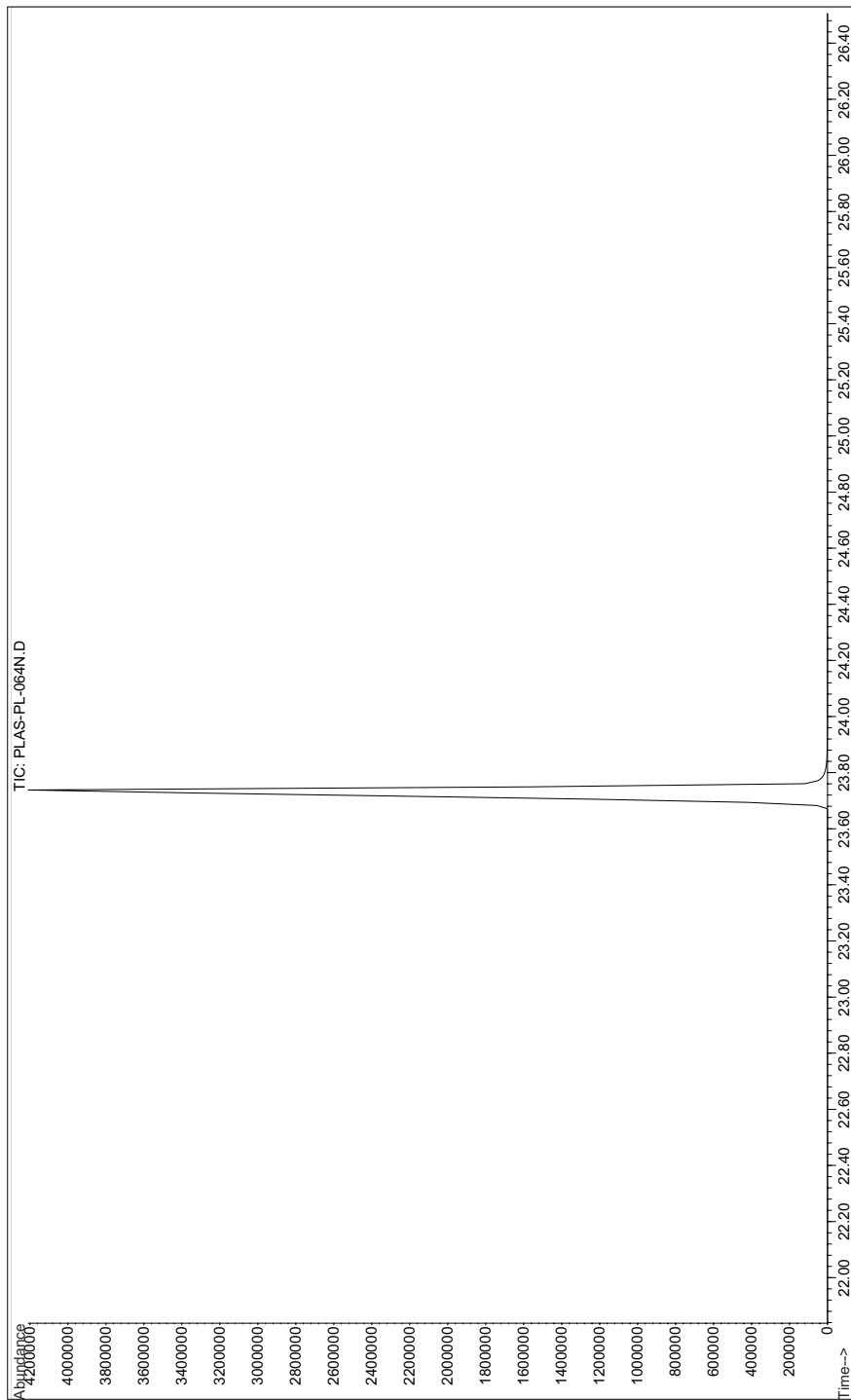
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

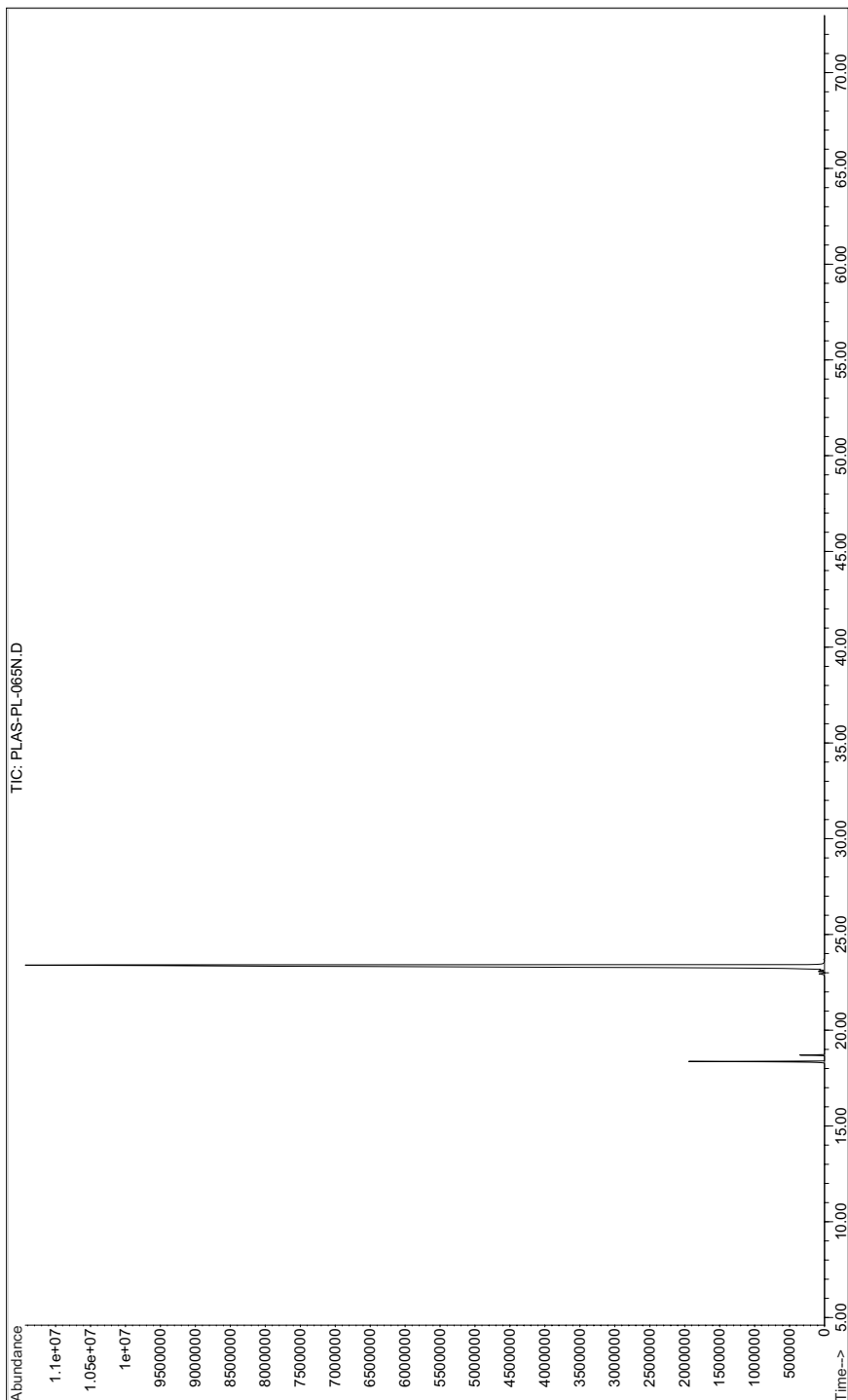


Analytical Information

Chromatogram for 2-Ethylhexyl sebacate - PLAS-PL-064

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

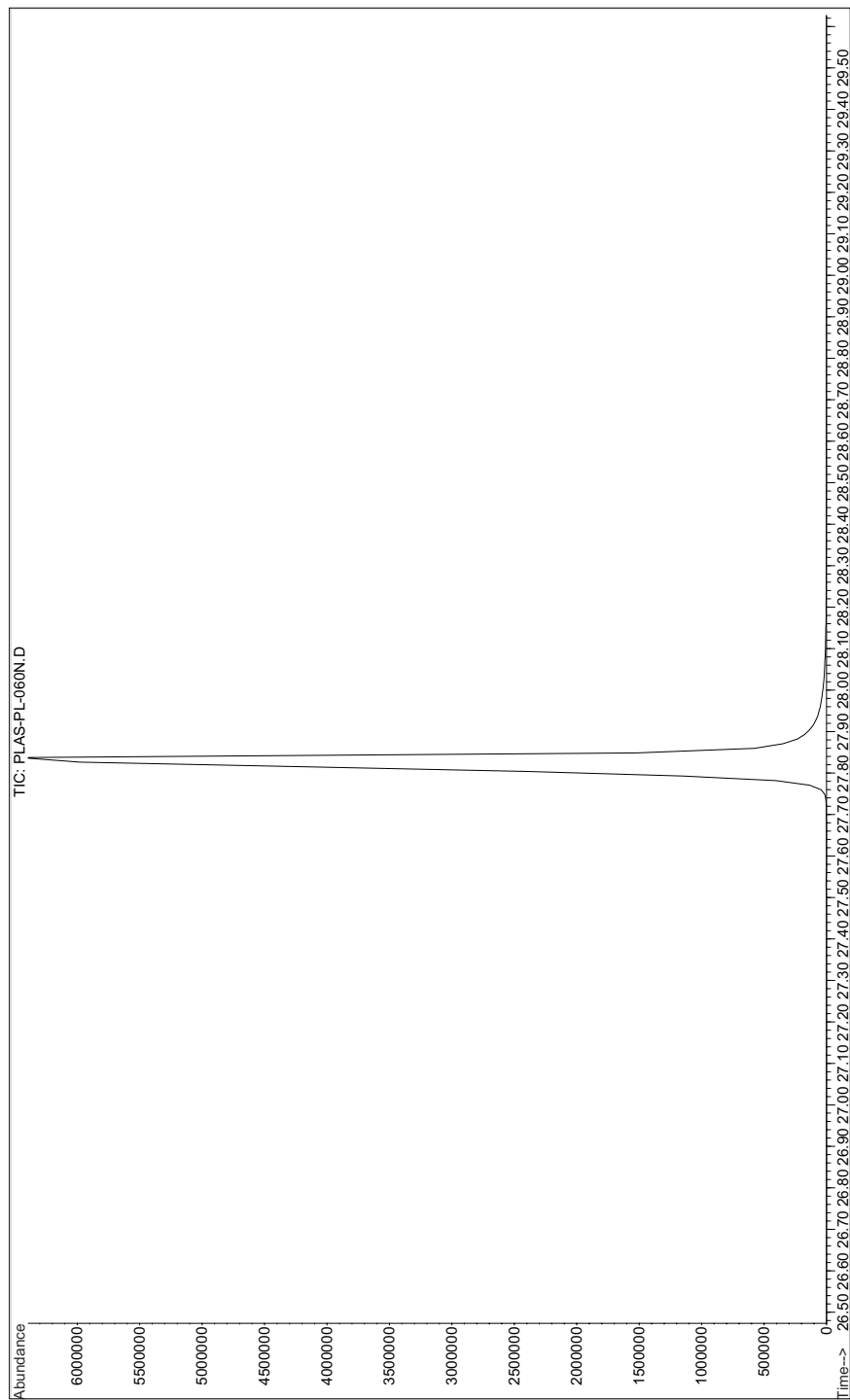


*Analytical Information***Chromatogram for *bis*(2-Ethylhexyl) terephthalate - PLAS-PL-065****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *Tris(2-ethylhexyl) Trimellitate - PLAS-PL-060*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

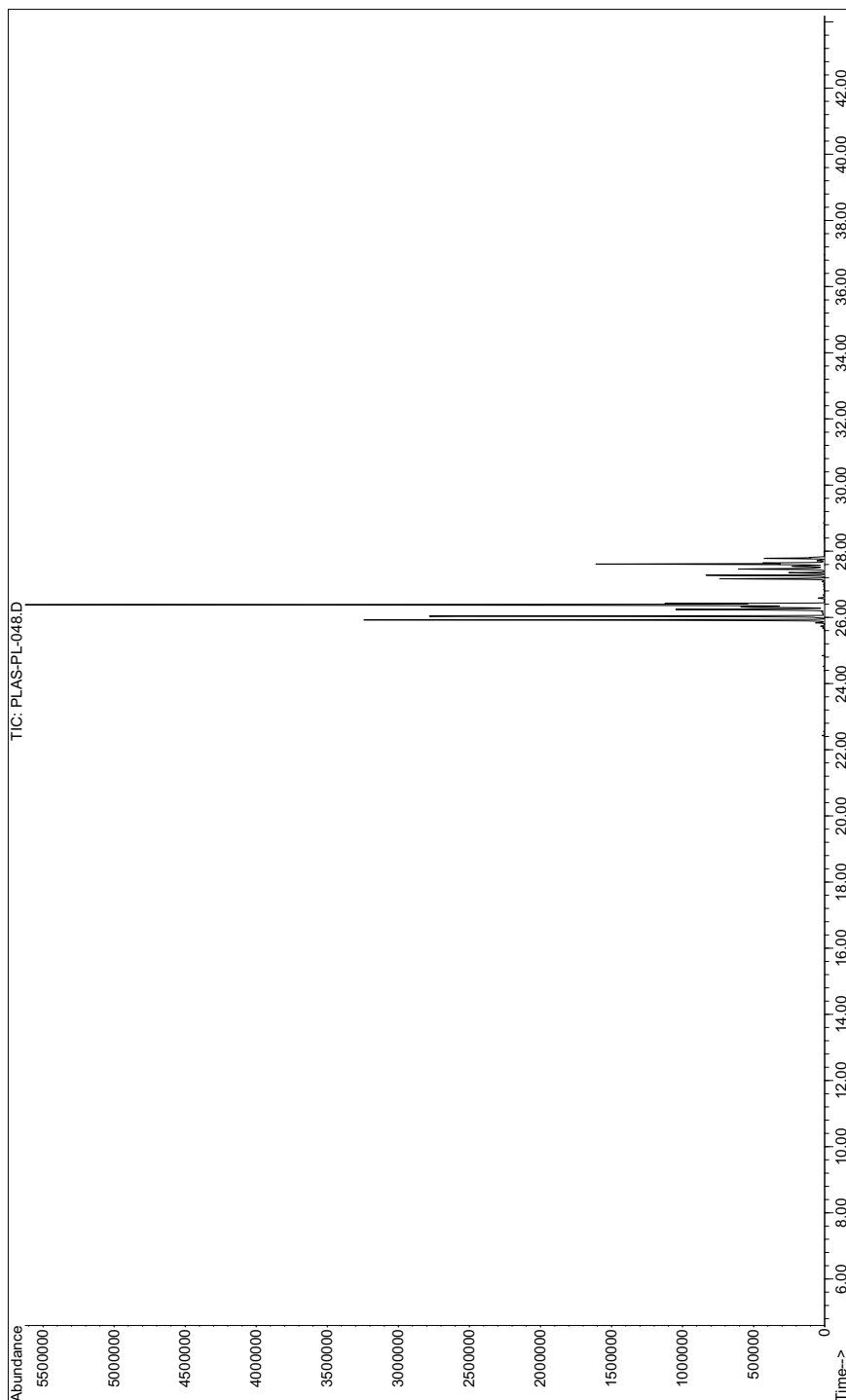


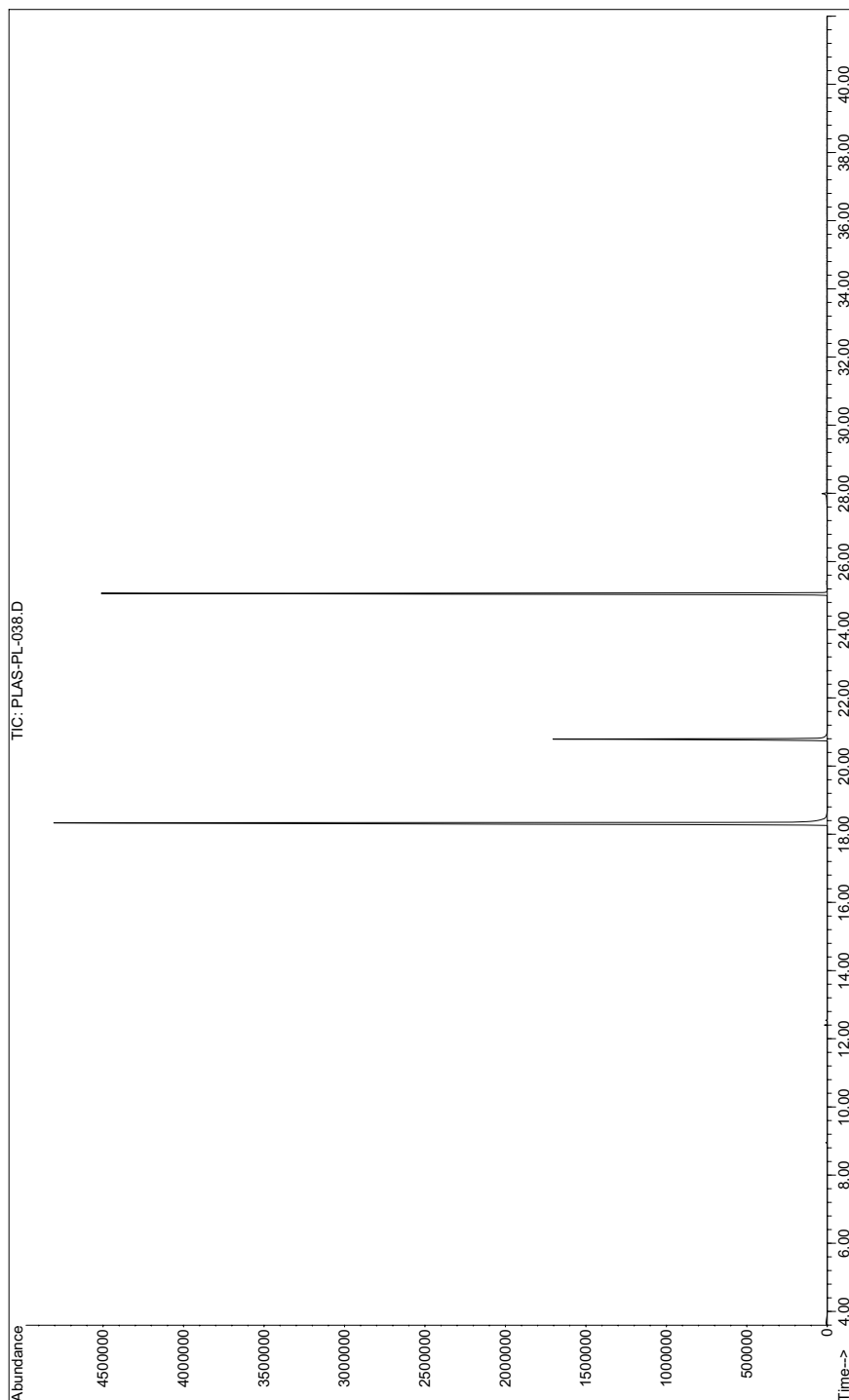
Analytical Information

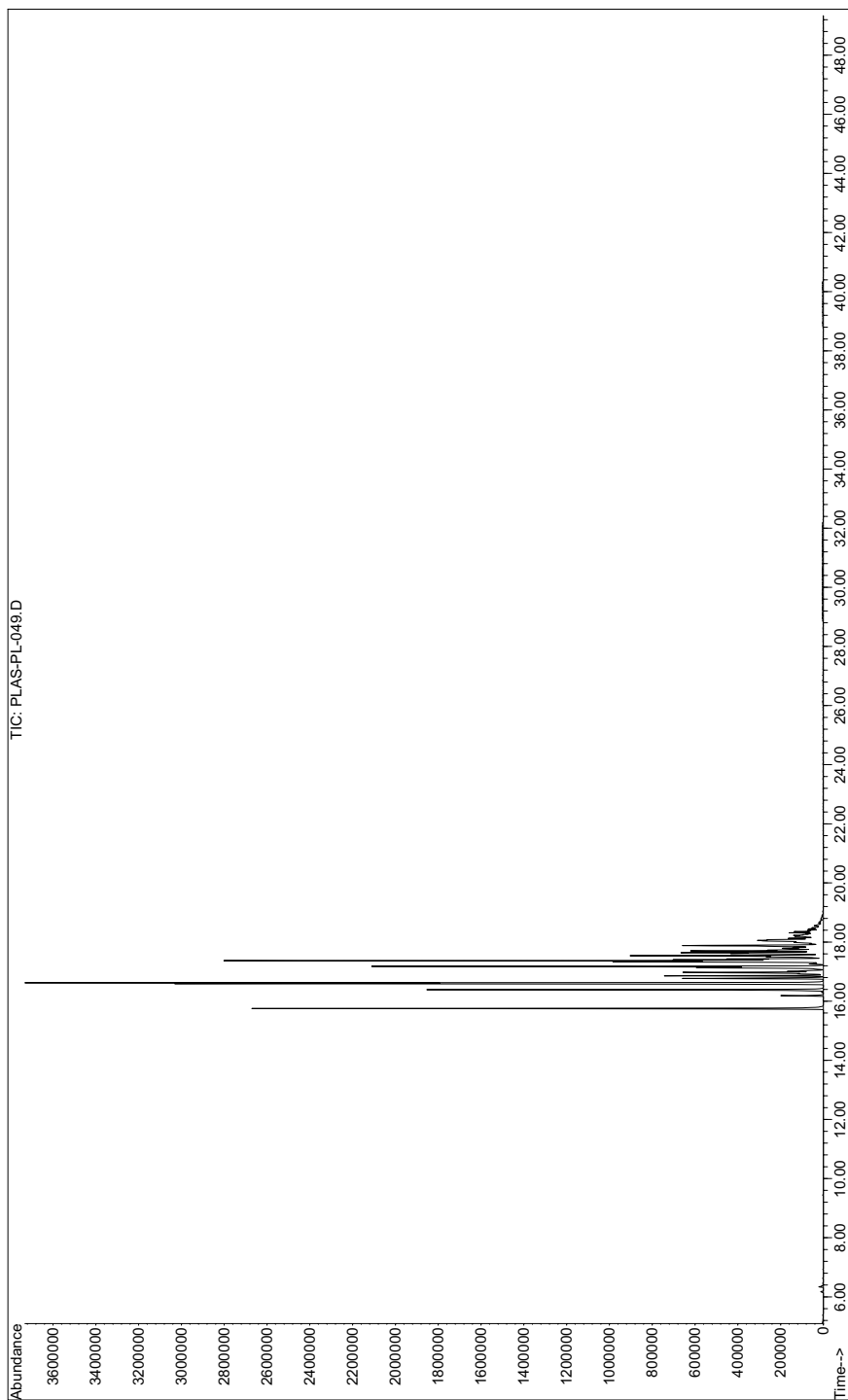
Chromatogram for *Flexol EP-8 - PLAS-PL-048*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD

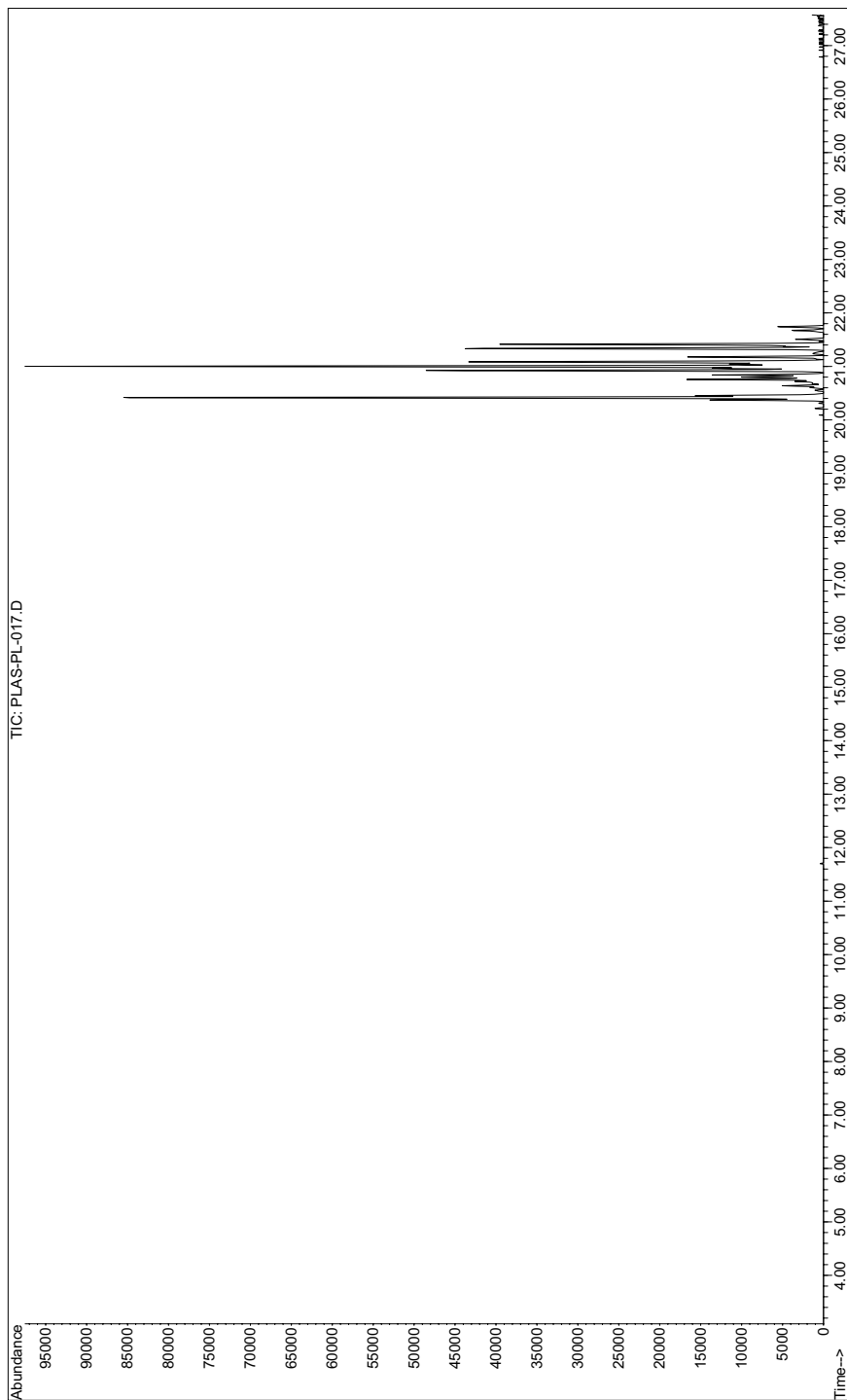


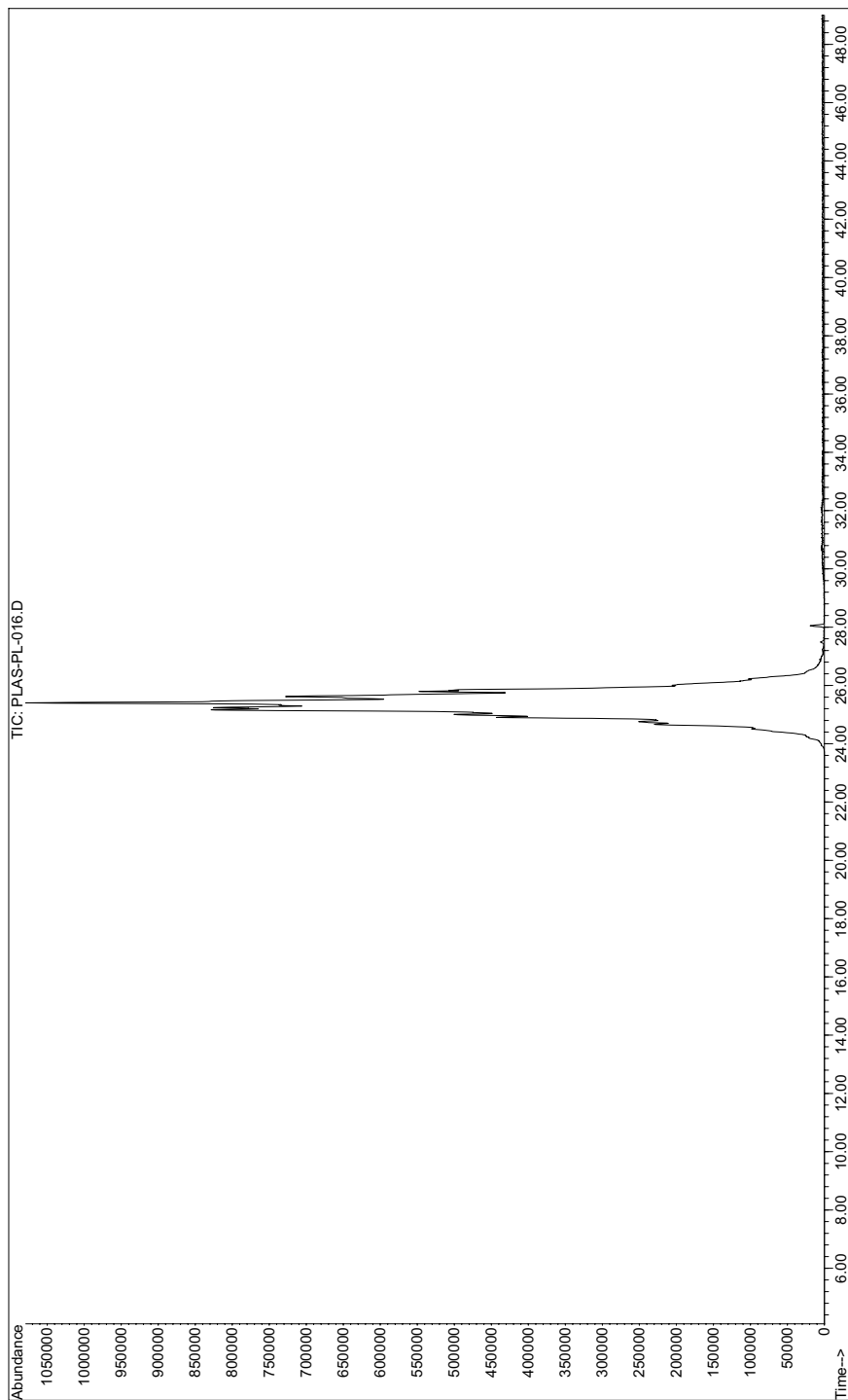
*Analytical Information***Chromatogram for *Hercoflex*[®] 900 - PLAS-PL-038****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

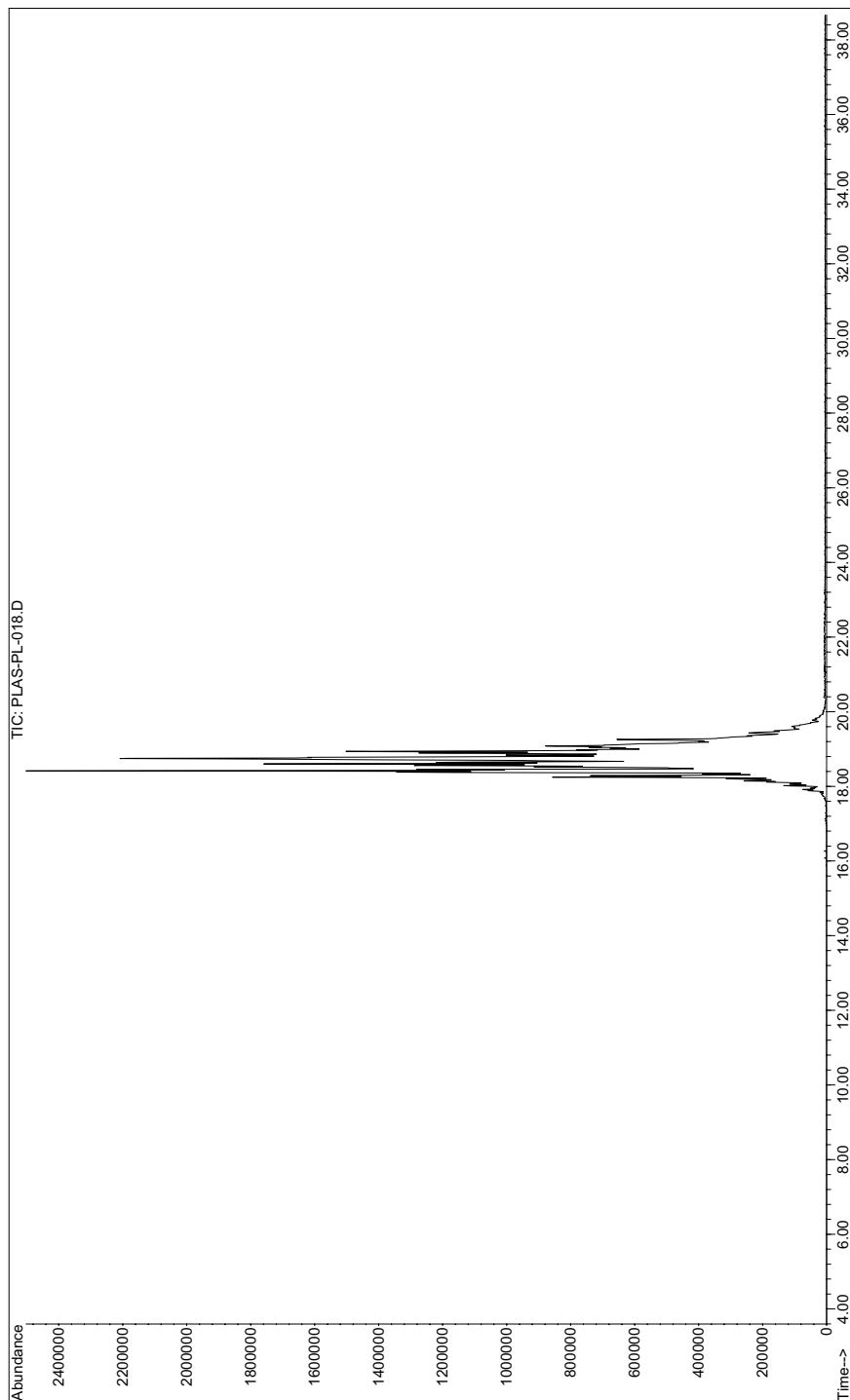
*Analytical Information***Chromatogram for *Imol S-140 - PLAS-PL-049*****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

*Analytical Information***Chromatogram for Jayflex[®] 77 - PLAS-PL-017****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD



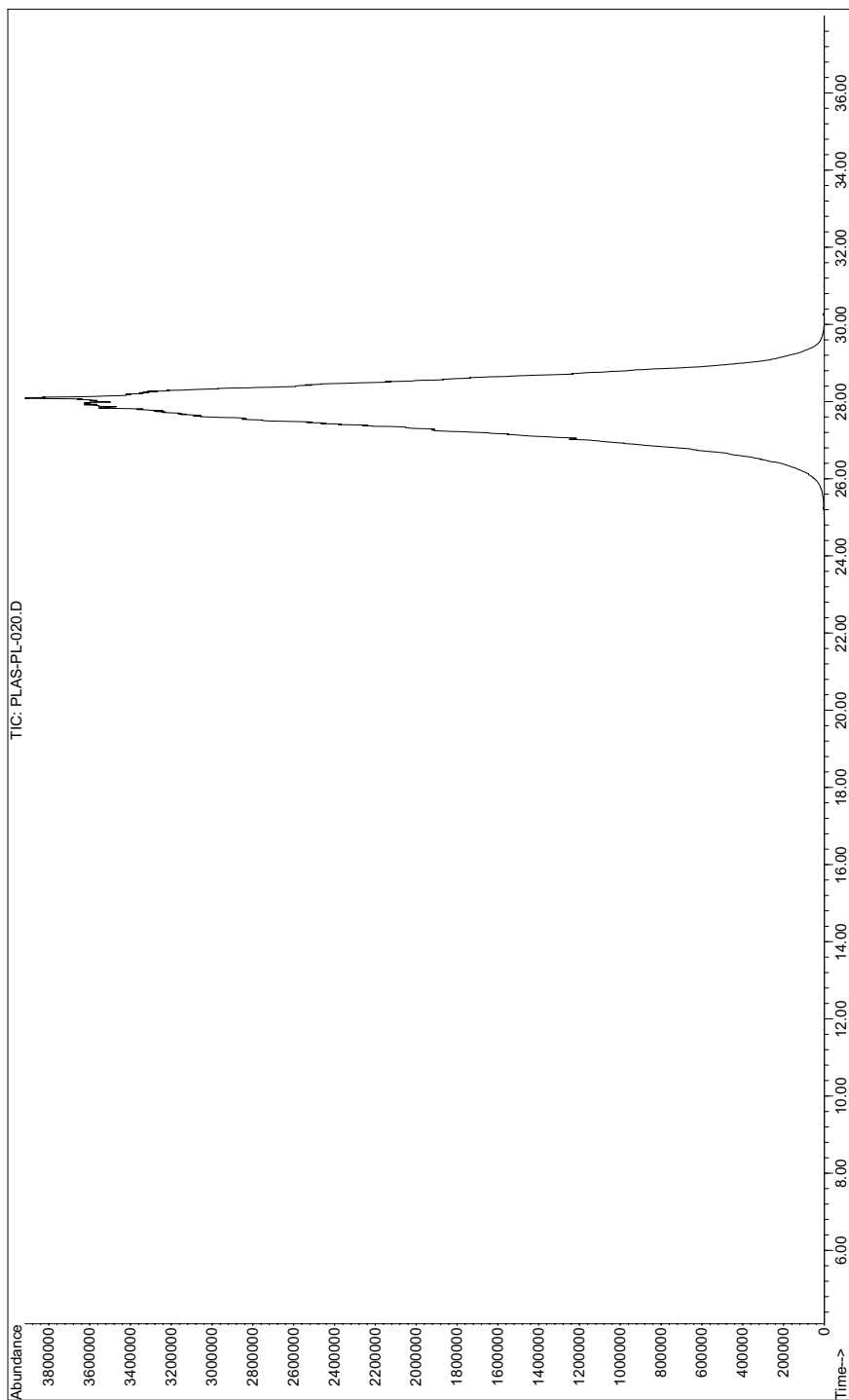
*Analytical Information***Chromatogram for Jayflex[®] DIDP - PLAS-PL-016****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

*Analytical Information***Chromatogram for Jayflex® DINP Plasticizer - PLAS-PL-018****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

Analytical Information

Chromatogram for Jayflex[®] DTDP plasticizer - PLAS-PL-020

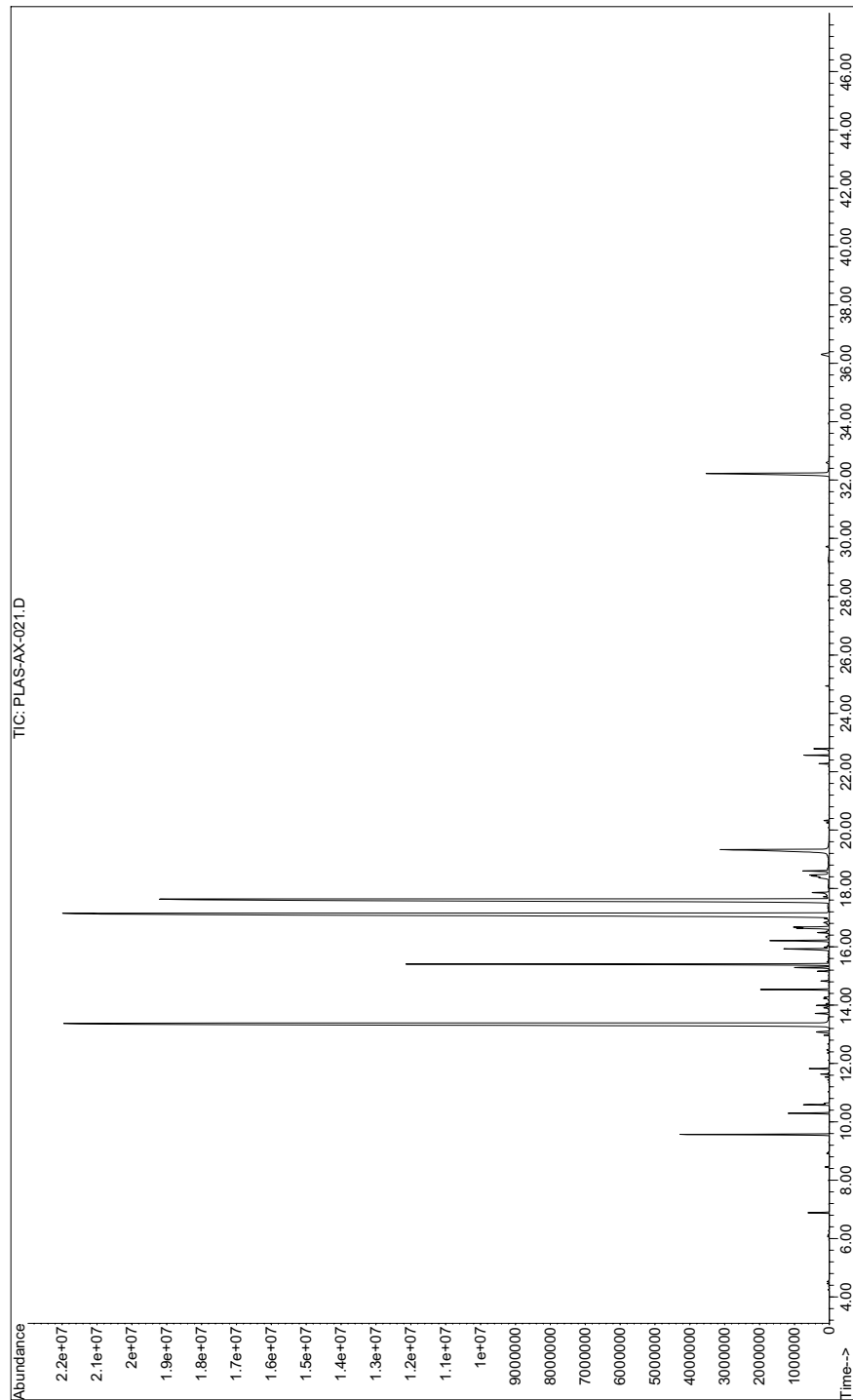
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD

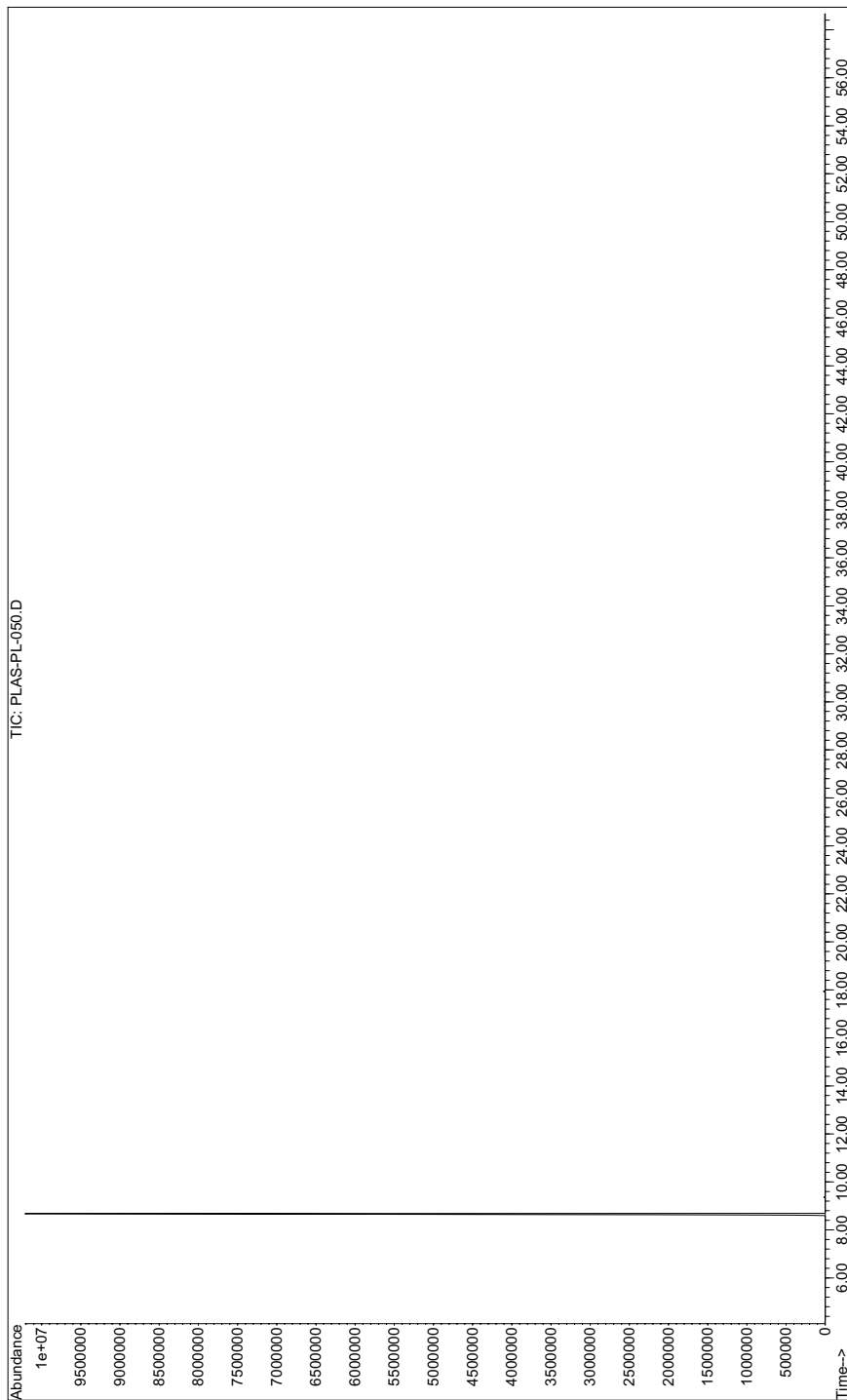


Analytical Information

Chromatogram for Jayflex® L11P-E Plasticizer - PLAS-PL-021

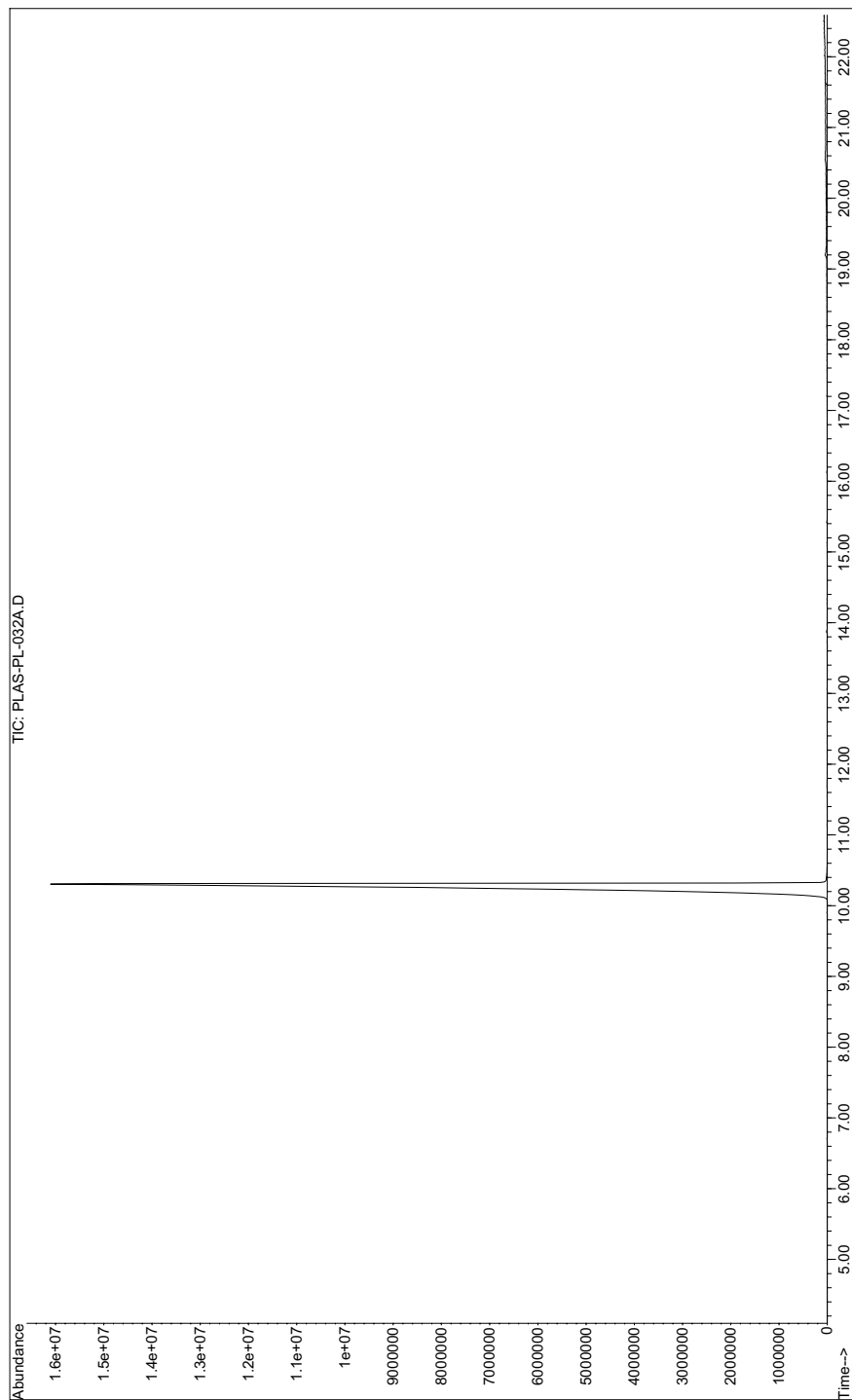
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



*Analytical Information***Chromatogram for Kesscoflex TRA - PLAS-PL-050****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

Mass Spectra for Laurex® - PLAS-PL-032

60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD

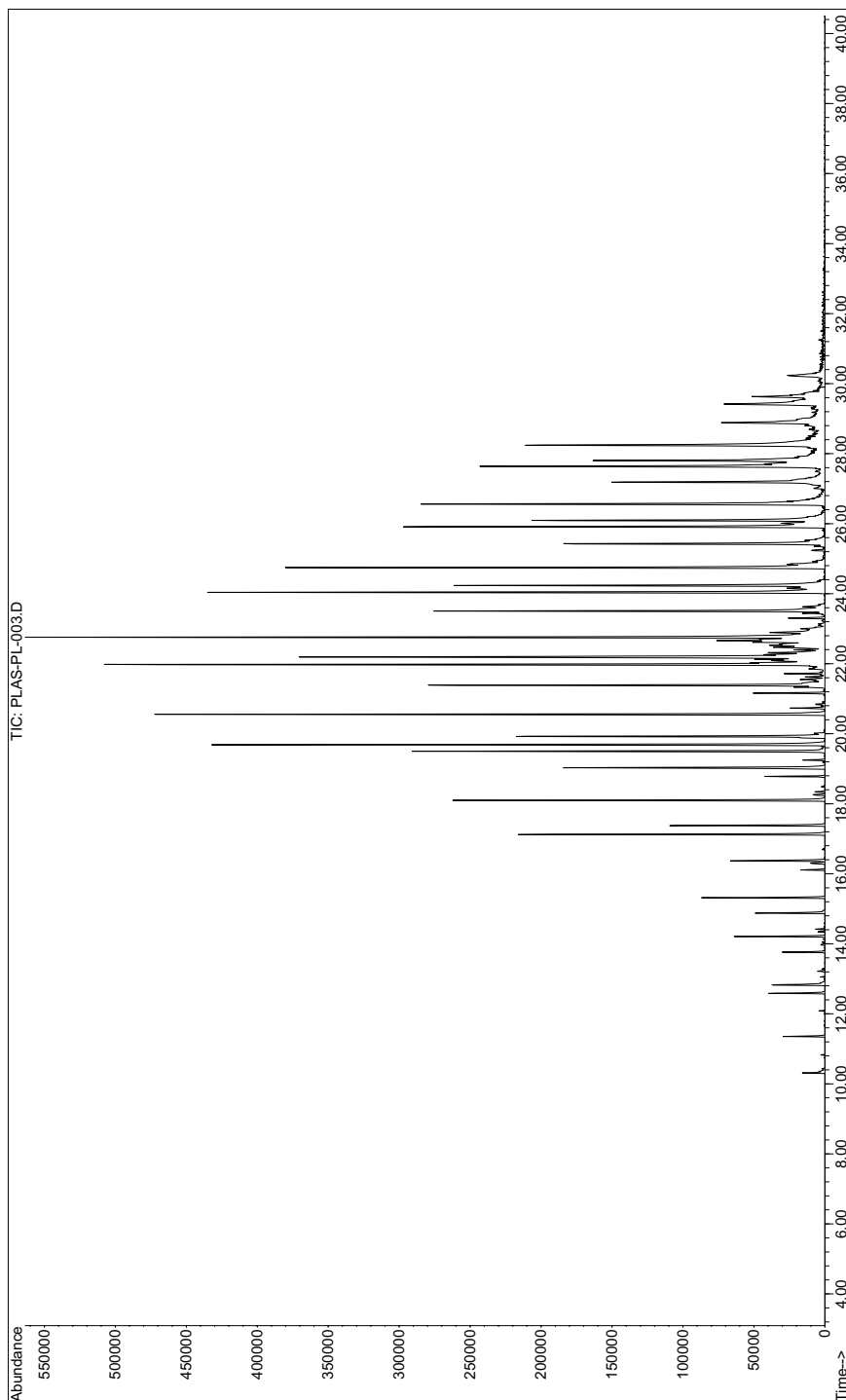


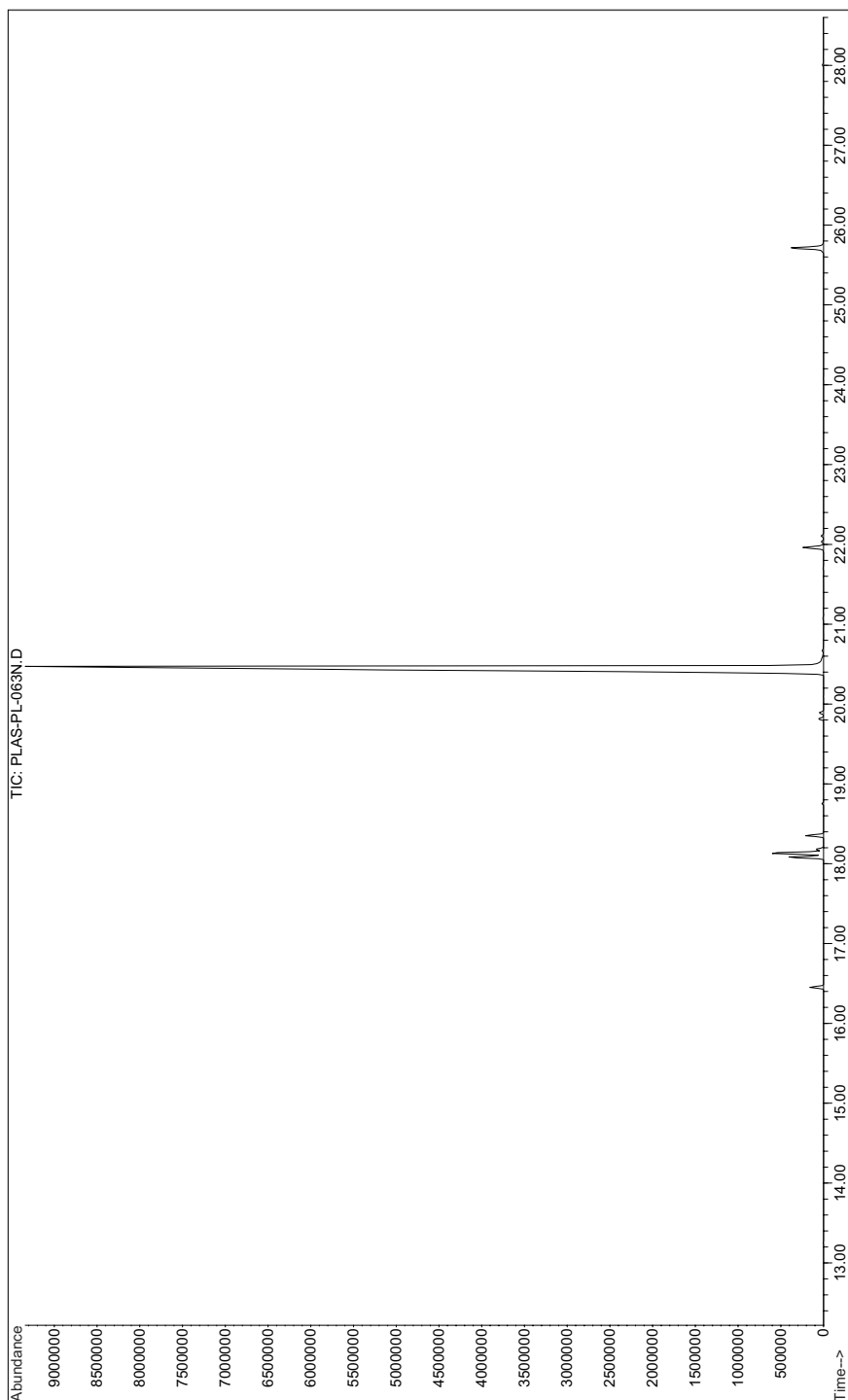
Analytical Information

Chromatogram for *Markstat*[®] 51 - PLAS-PL-003

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

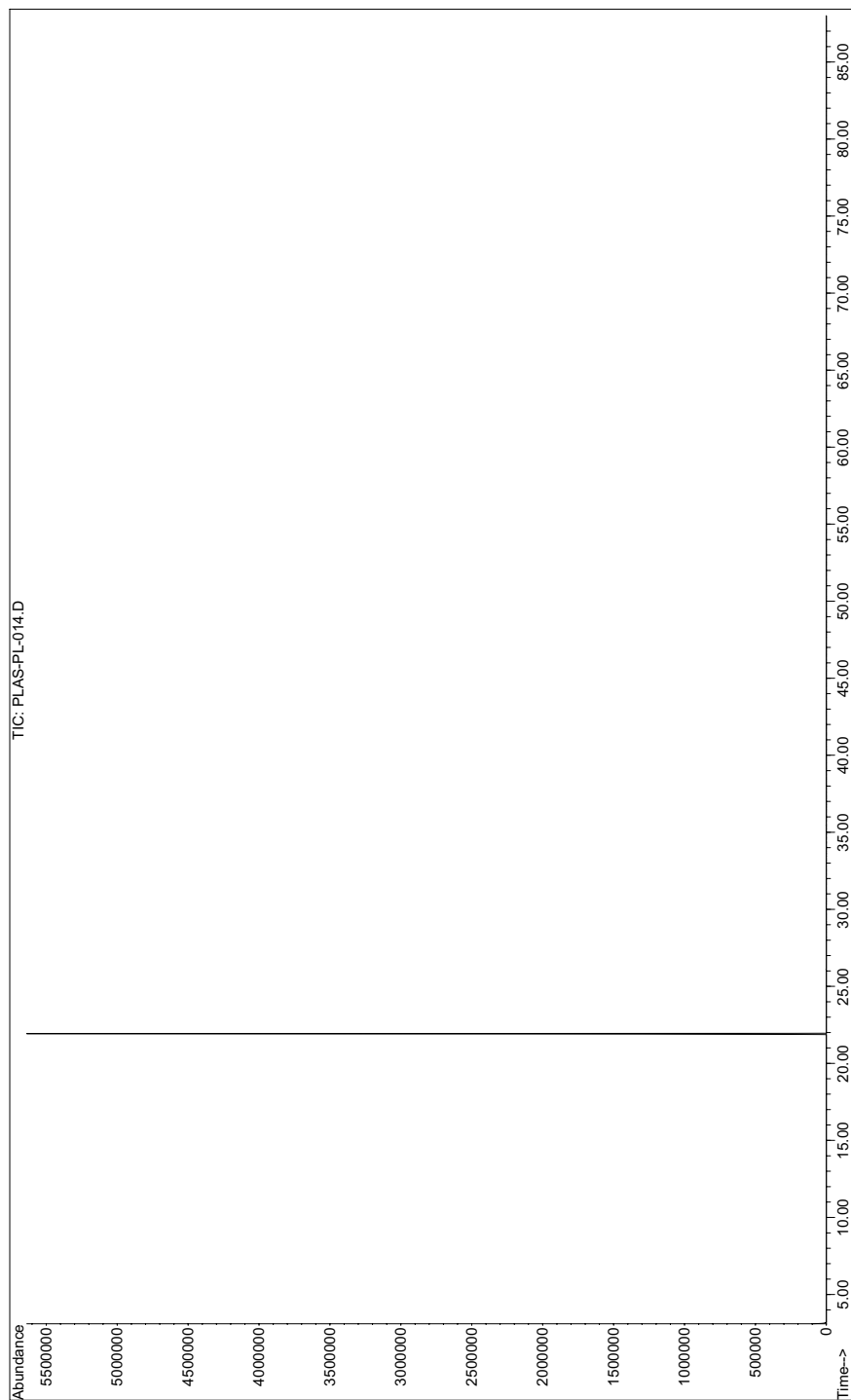
Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *Methyl O-Acetylricinoleate* - PLAS-PL-063****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

*Analytical Information***Chromatogram for Morflex[®] 150 - PLAS-PL-014****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

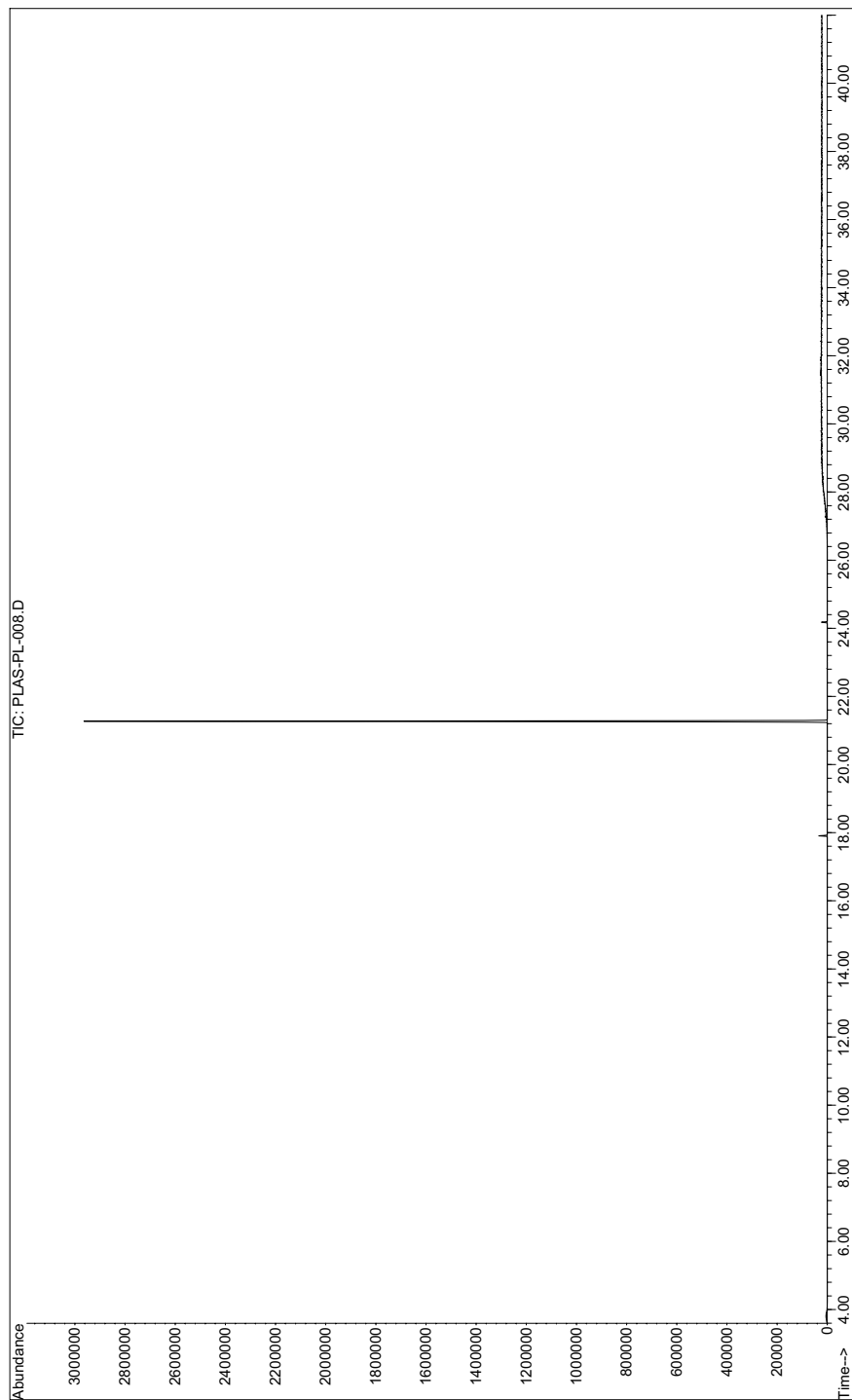
Inj Temp=250 °C, Det=MSD

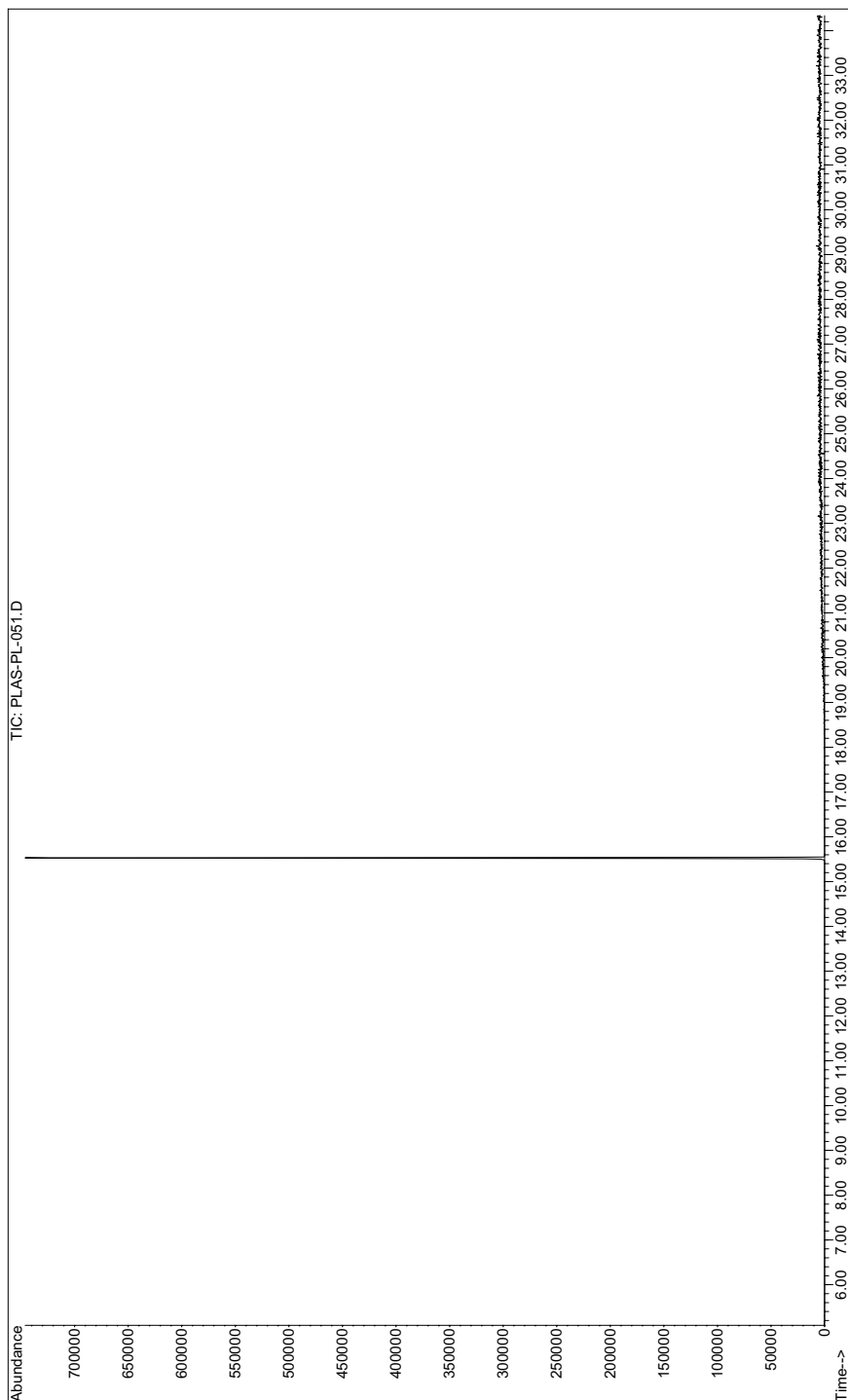


Analytical Information

Chromatogram for*Morflex® 190 - PLAS-PL-008*

Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

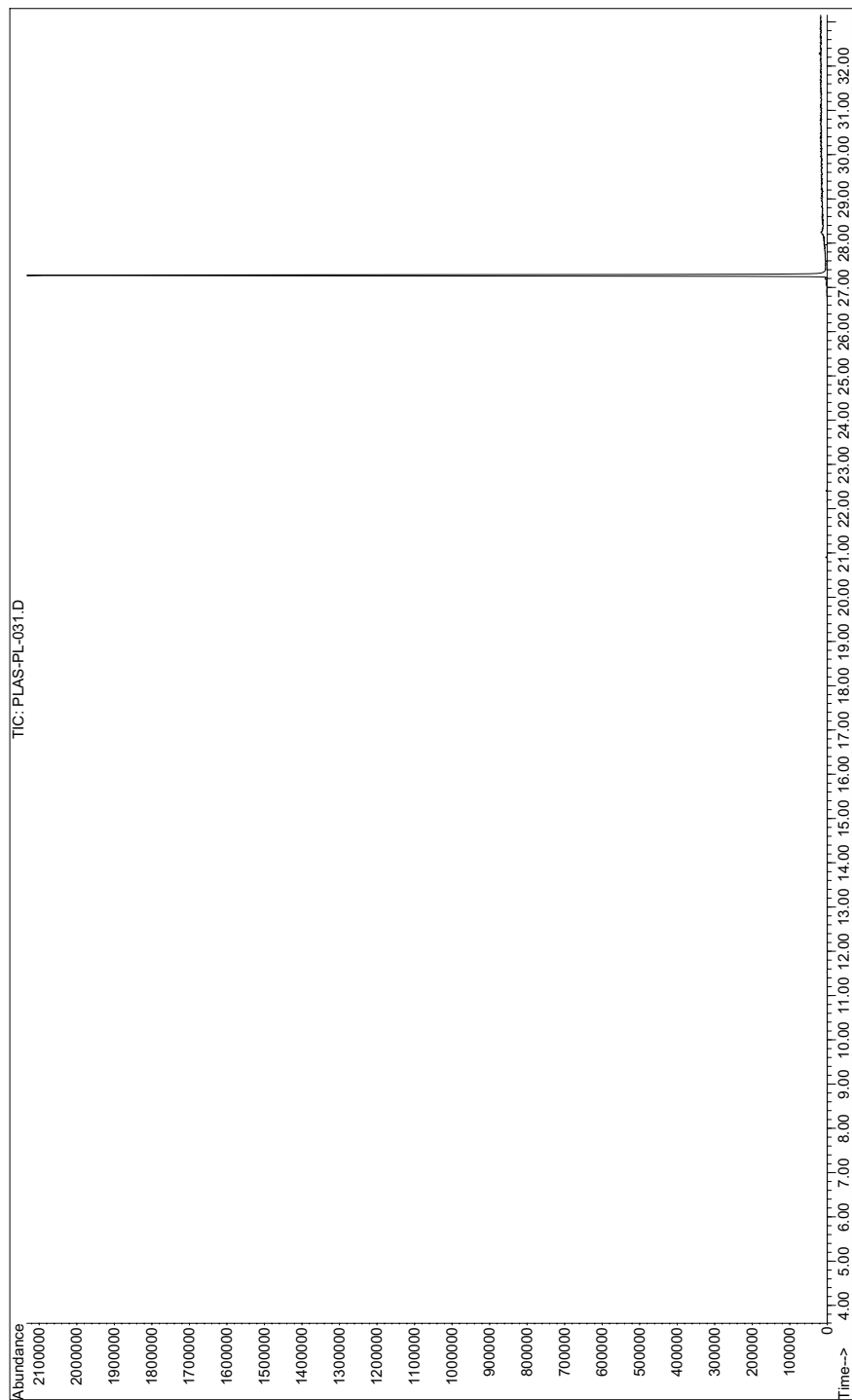


*Analytical Information***Chromatogram for Morflex[®] 310 - PLAS-PL-051****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

Analytical Information

Chromatogram for*Morflex*[®] 560 - PLAS-PL-031

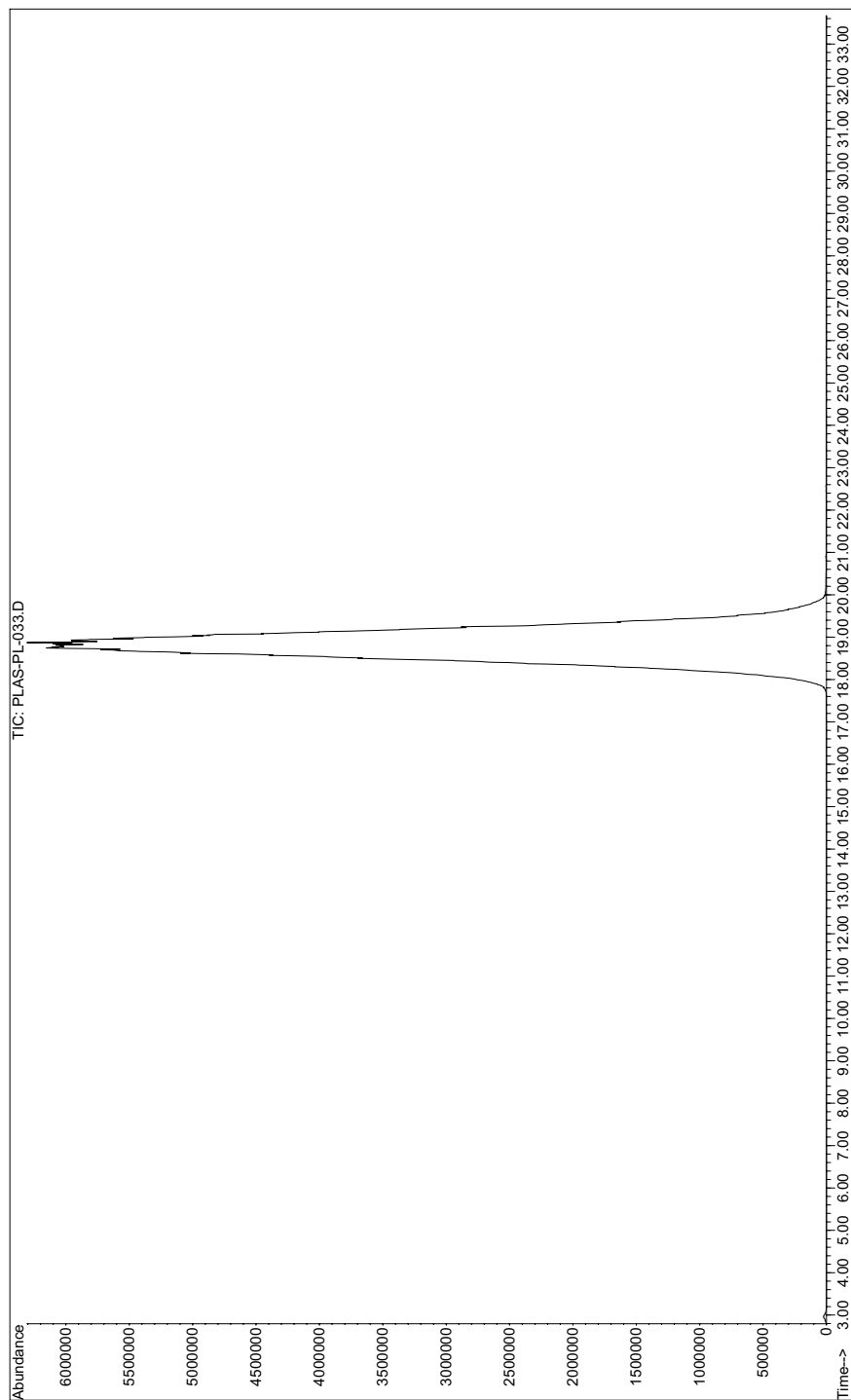
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

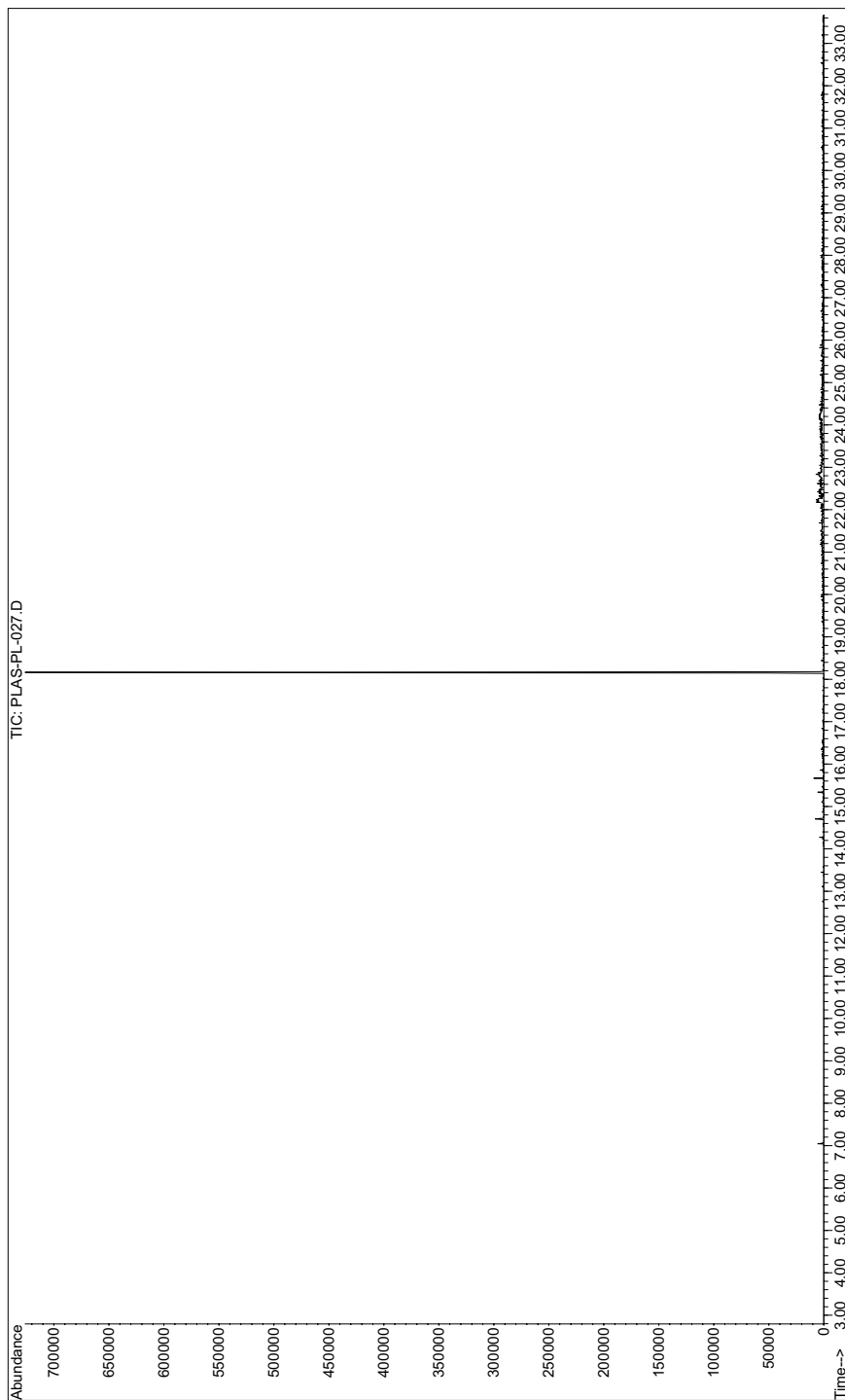


Analytical Information

Chromatogram for *Morflex*[®] *x-1125* - *PLAS-PL-033*

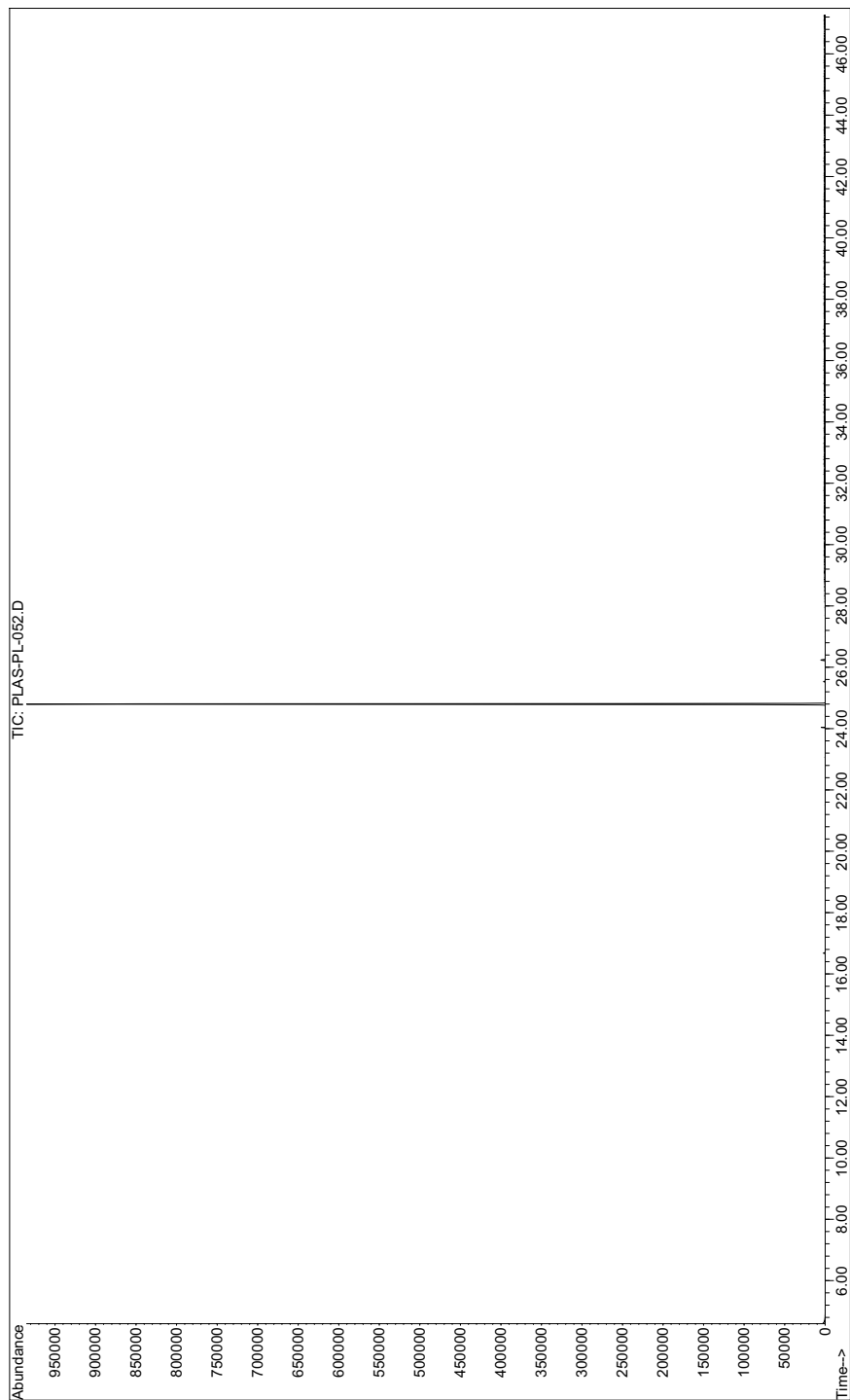
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



*Analytical Information***Chromatogram for *Paraplex*[®] G-30 - PLAS-PL-027****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

*Analytical Information***Chromatogram for *Plasthall*[®] DOZ - PLAS-PL-052****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

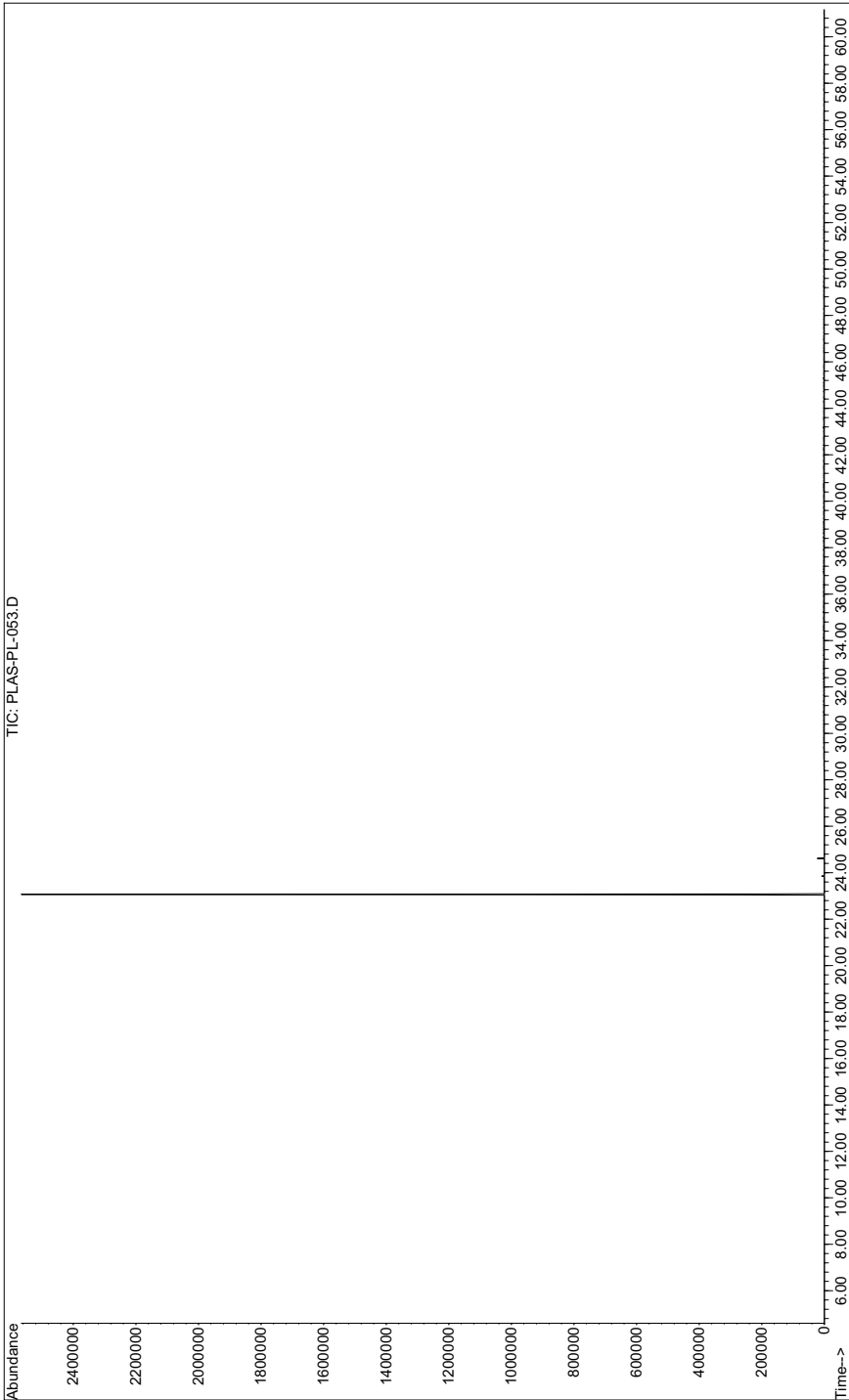
Inj Temp=250 °C, Det=MSD

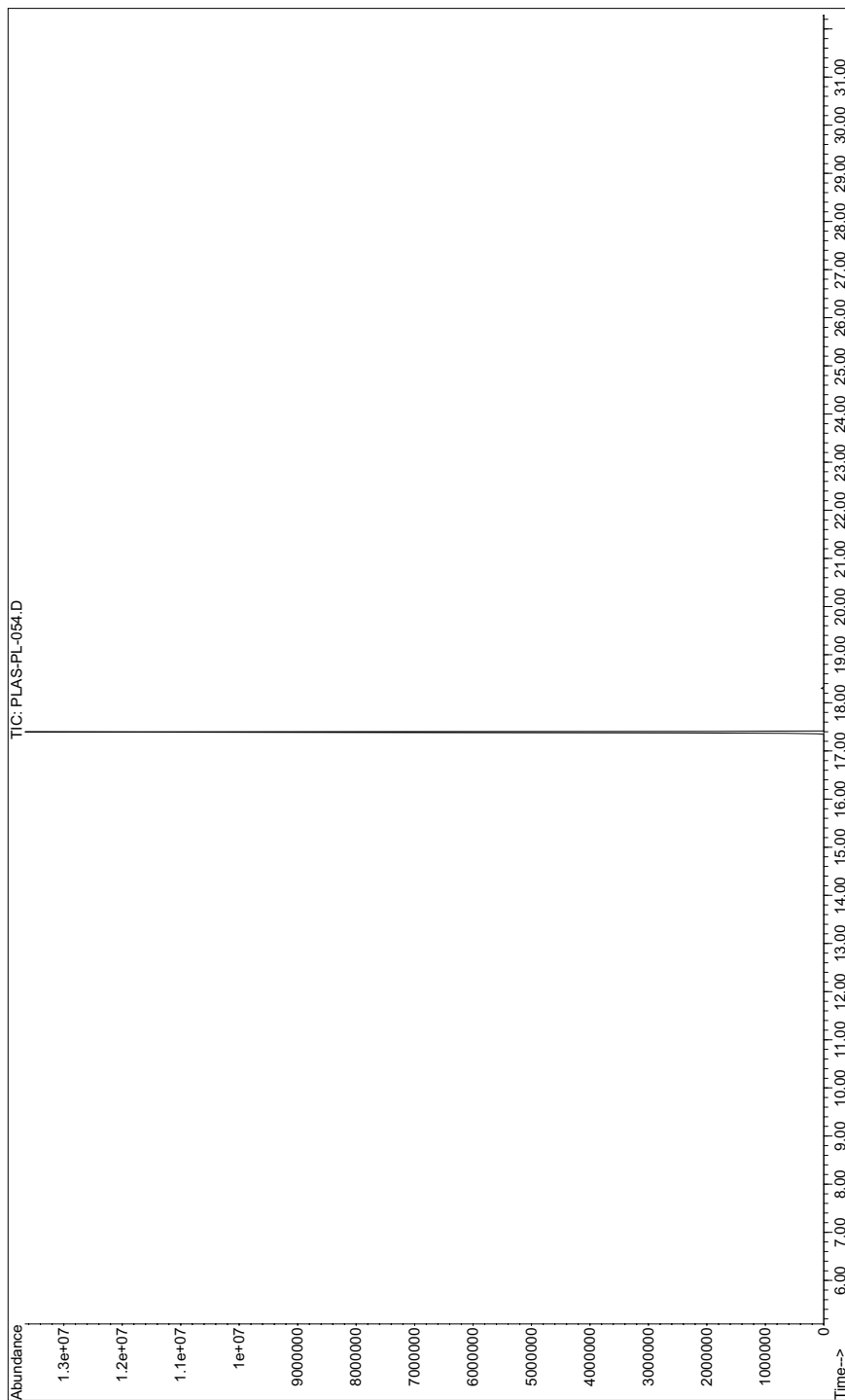


Analytical Information

Chromatogram for *Plastolein 9050 - PLAS-PL-053*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD

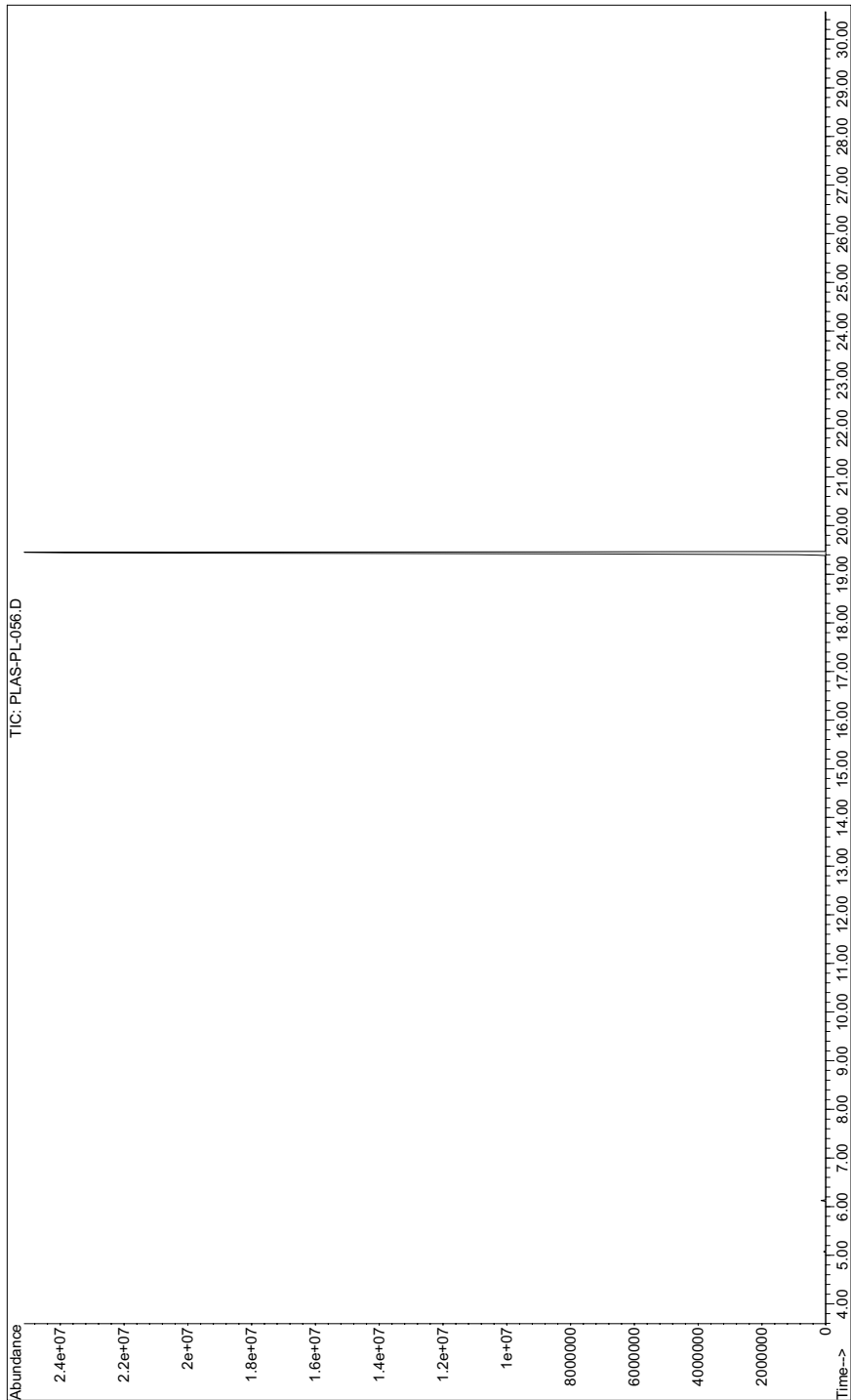


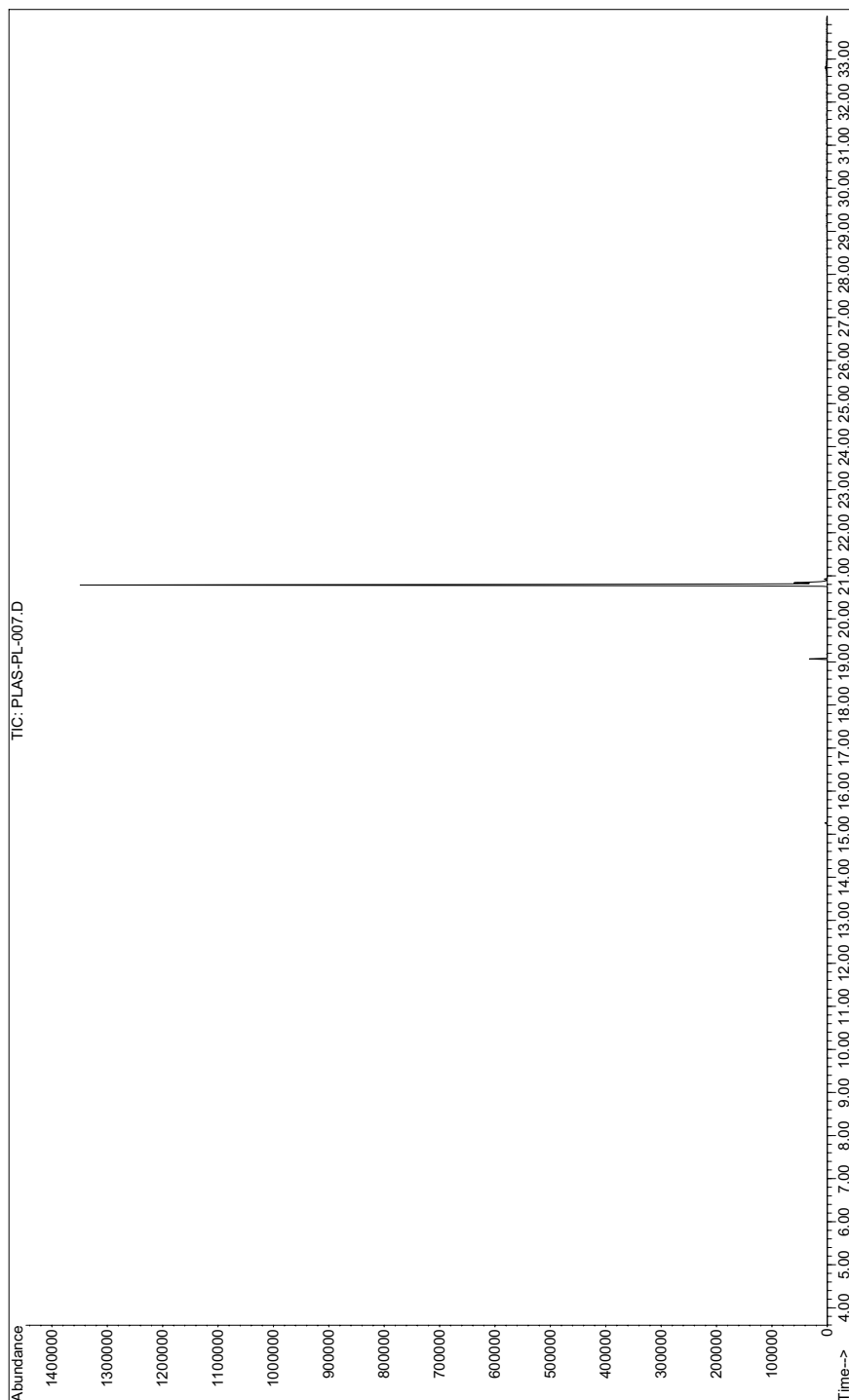
*Analytical Information***Chromatogram for Polycizer[®] 162 - PLAS-PL-054****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

Analytical Information

Chromatogram for Polycizer[®] 632 - PLAS-PL-056

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

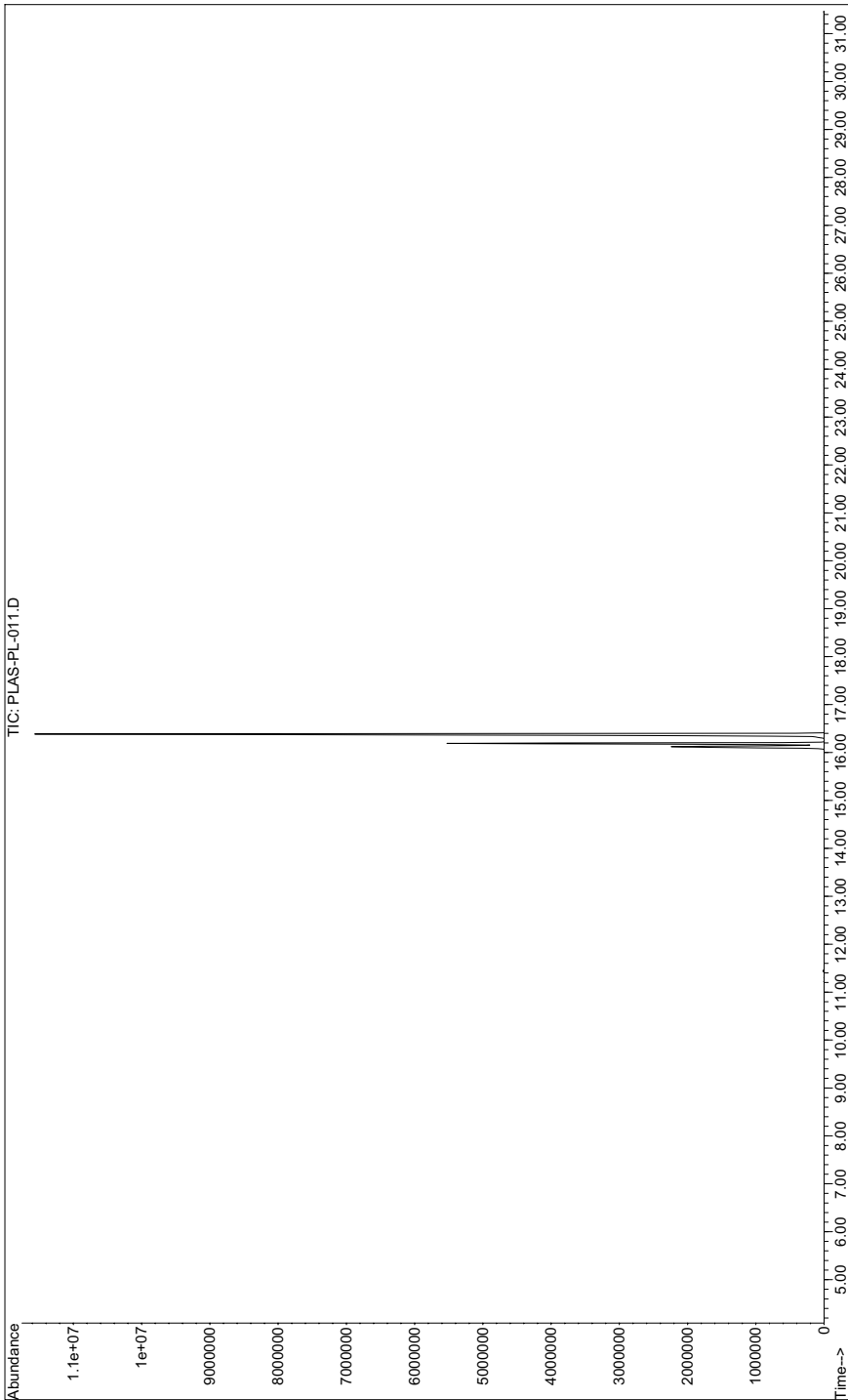


*Analytical Information***Chromatogram for Polycizer[®] Butyl Oleate - PLAS-PL-007****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

Analytical Information

Chromatogram for *Polycizer® DP 500 - PLAS-PL-011*

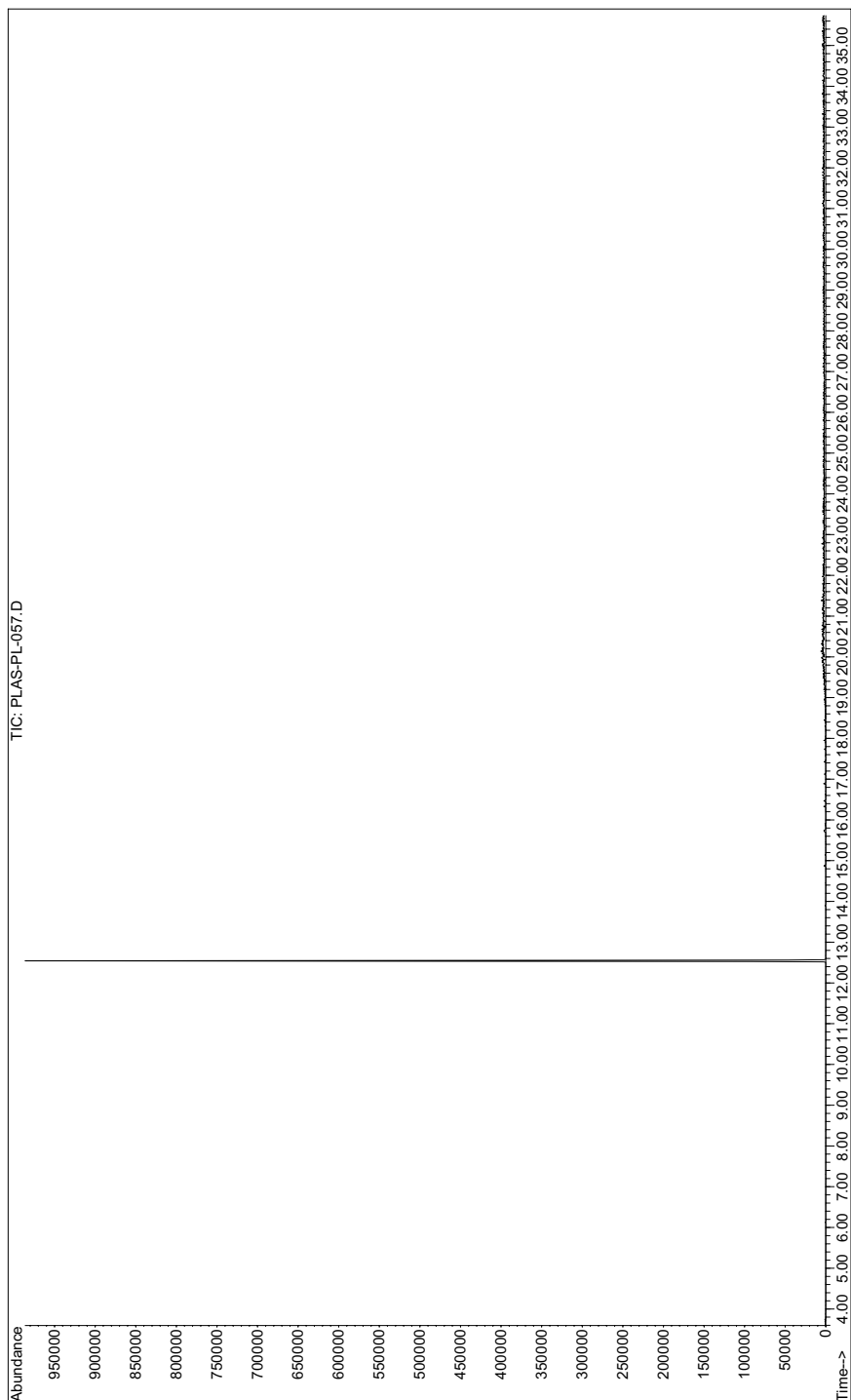
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

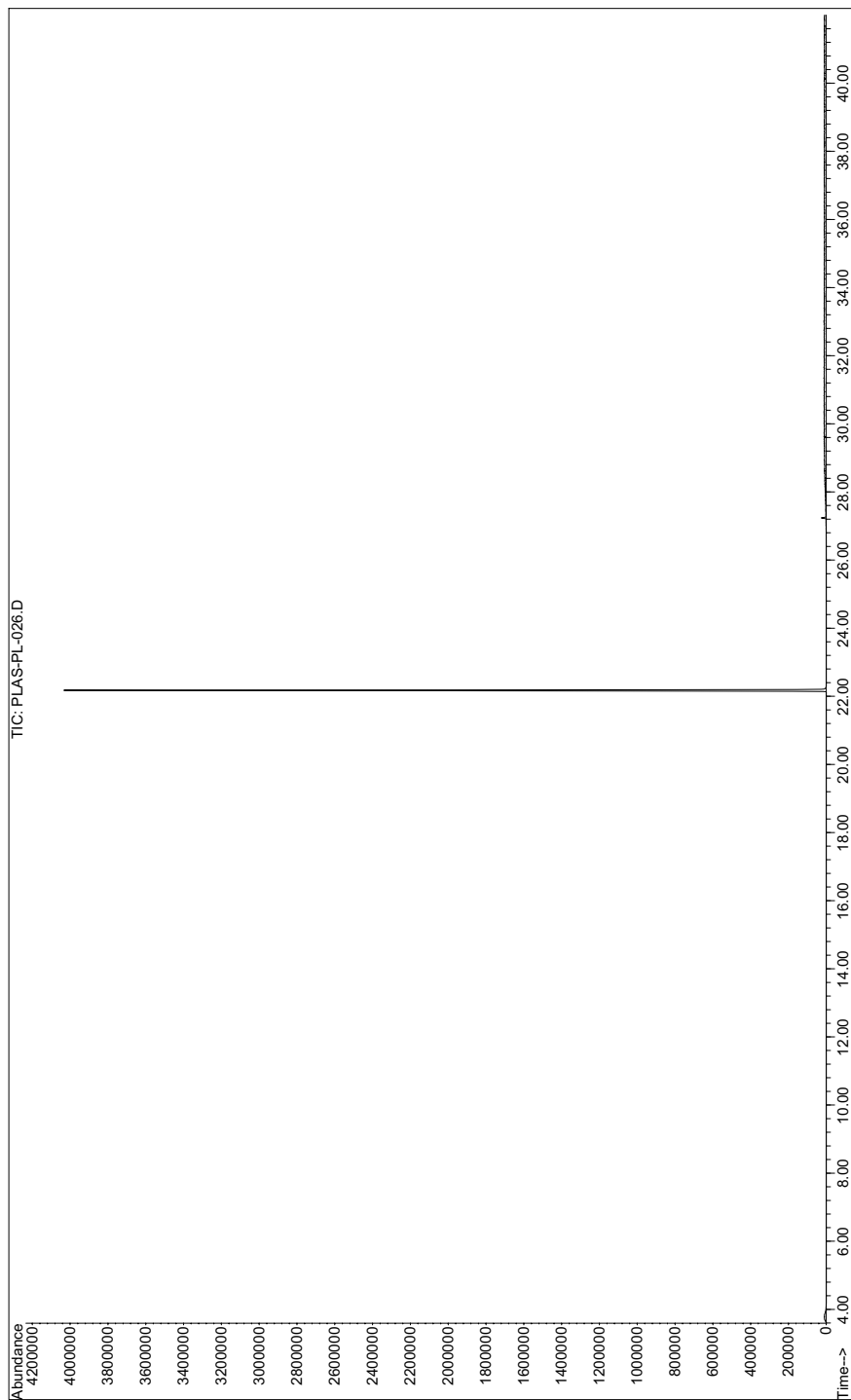


Analytical Information

Chromatogram for *Polycizer® W 260 - PLAS-PL-057*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min

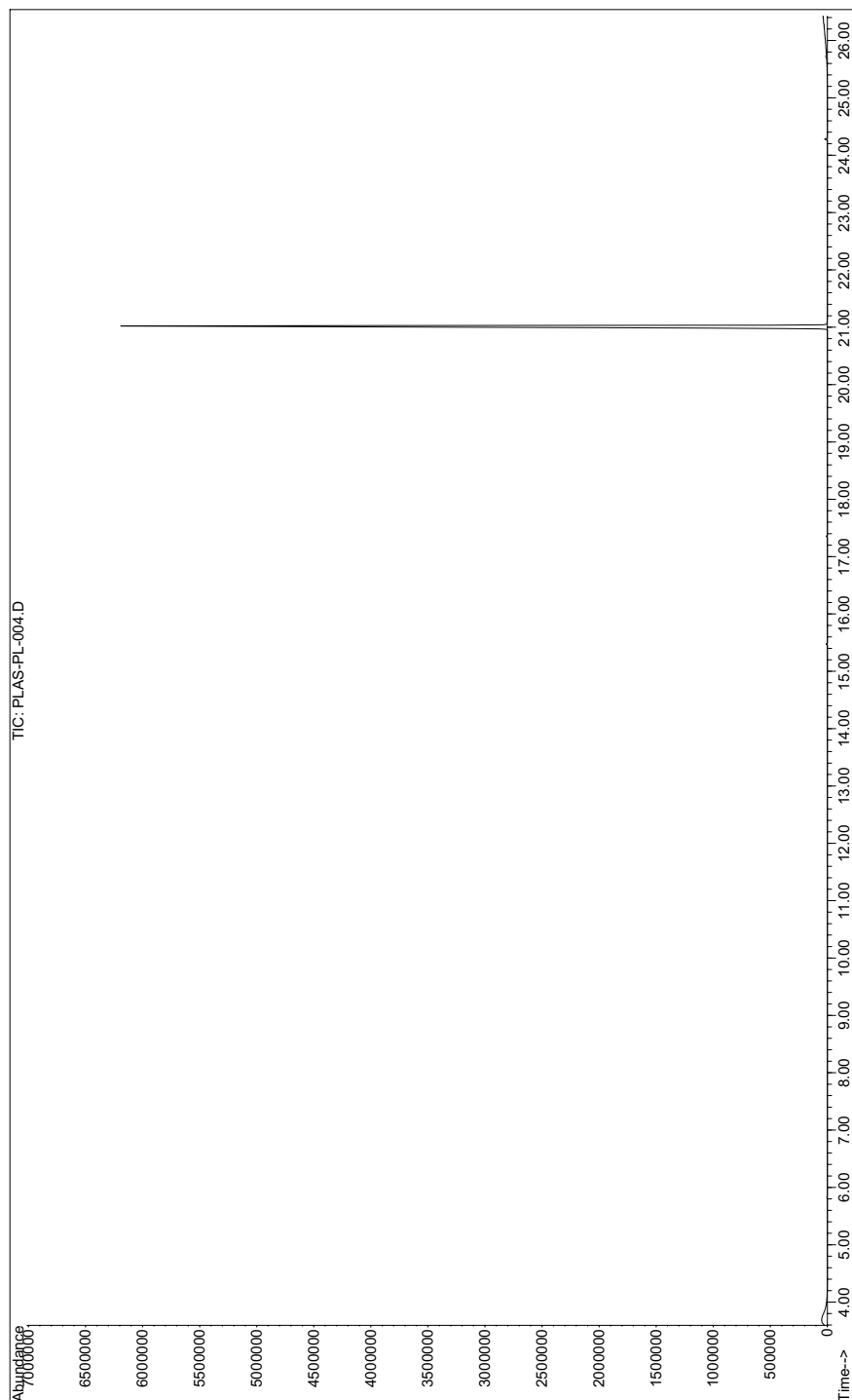


*Analytical Information***Chromatogram for *Santicizer*[®] 141 - PLAS-PL-026****Analytical Conditions Summary** 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD

Analytical Information

Chromatogram for *Santicizer*[®] 160 - PLAS-PL-004

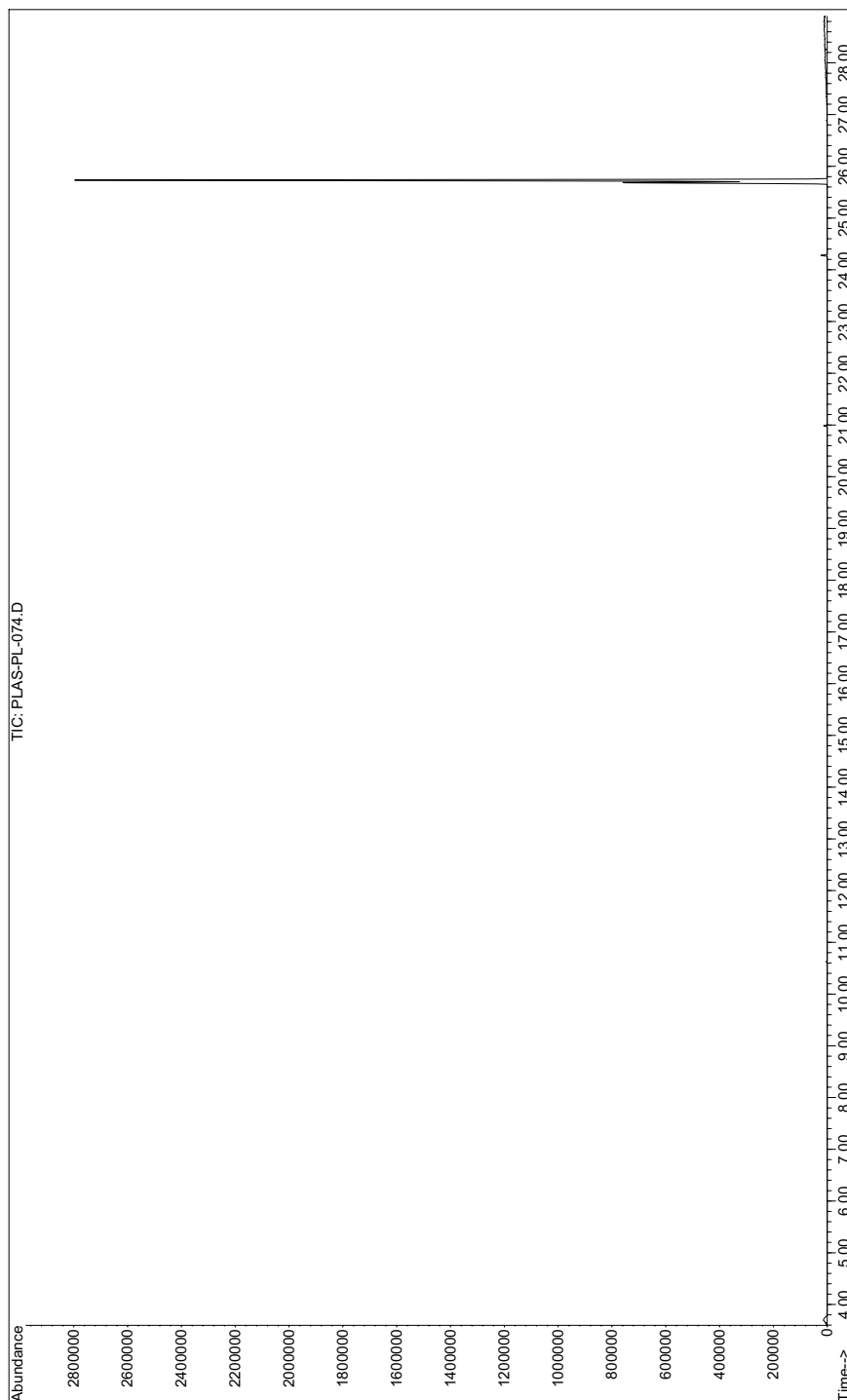
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Santicizer® 278 - PLAS-PL-074*

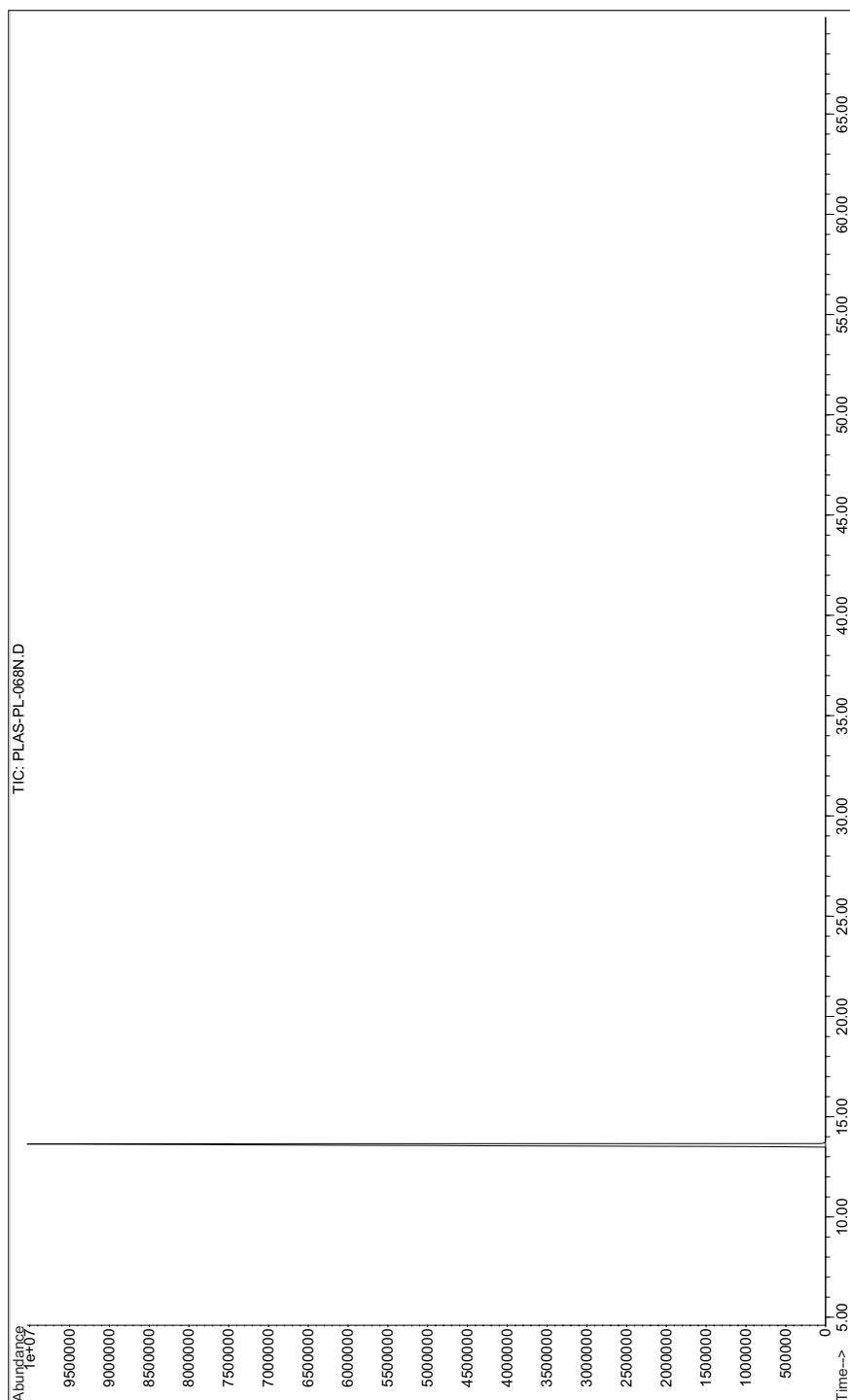
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Tributylphosphate - PLAS-PL-068*

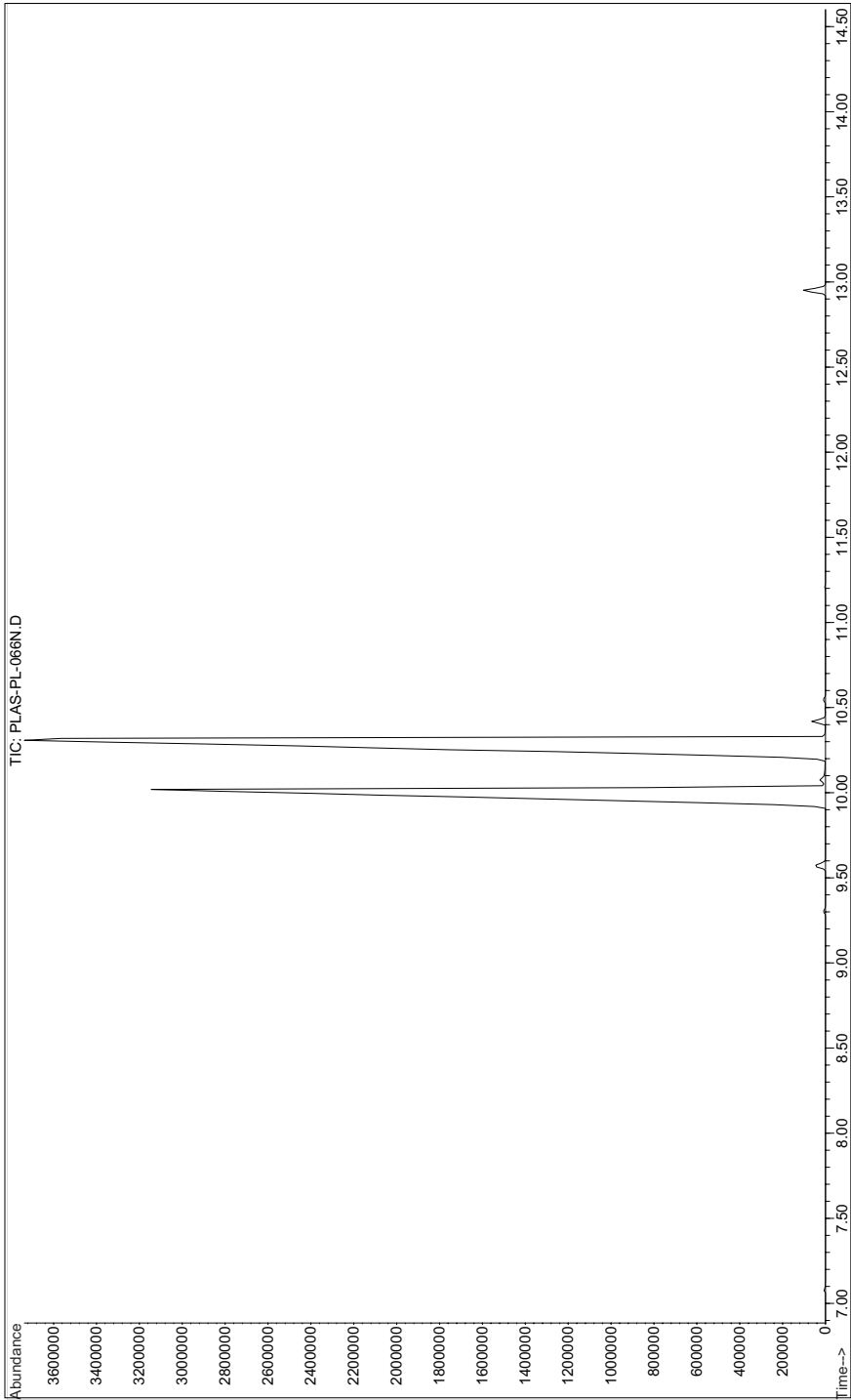
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

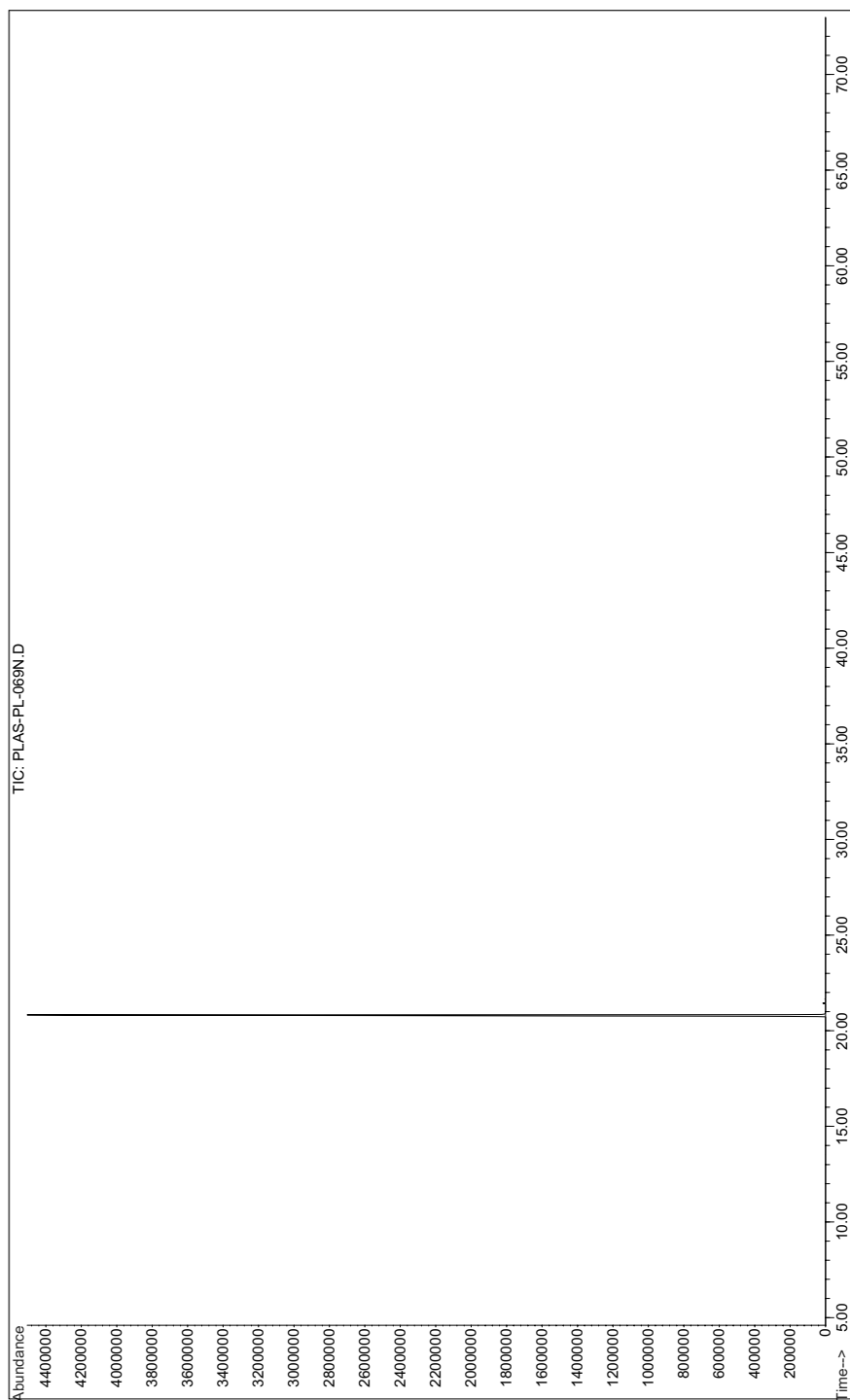


Analytical Information

Chromatogram for 2,2,4-Trimethyl-1,3-pentanediol-isobutyrate - PLAS-PL-066

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

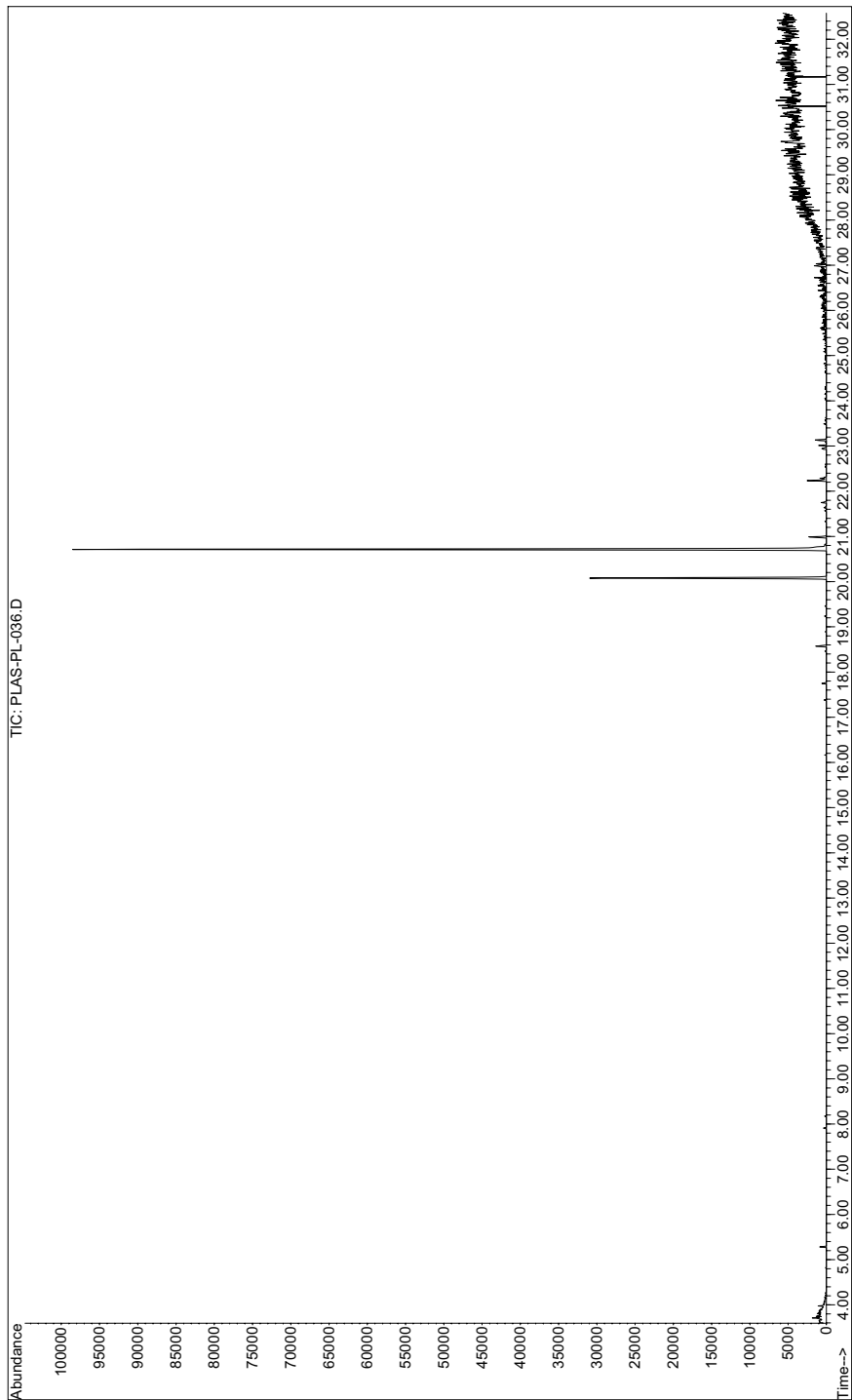


*Analytical Information***Chromatogram for Triphenylphosphate - PLAS-PL-069****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD

Analytical Information

Chromatogram for *Vinsol*[®] resin- PLAS-PL-036

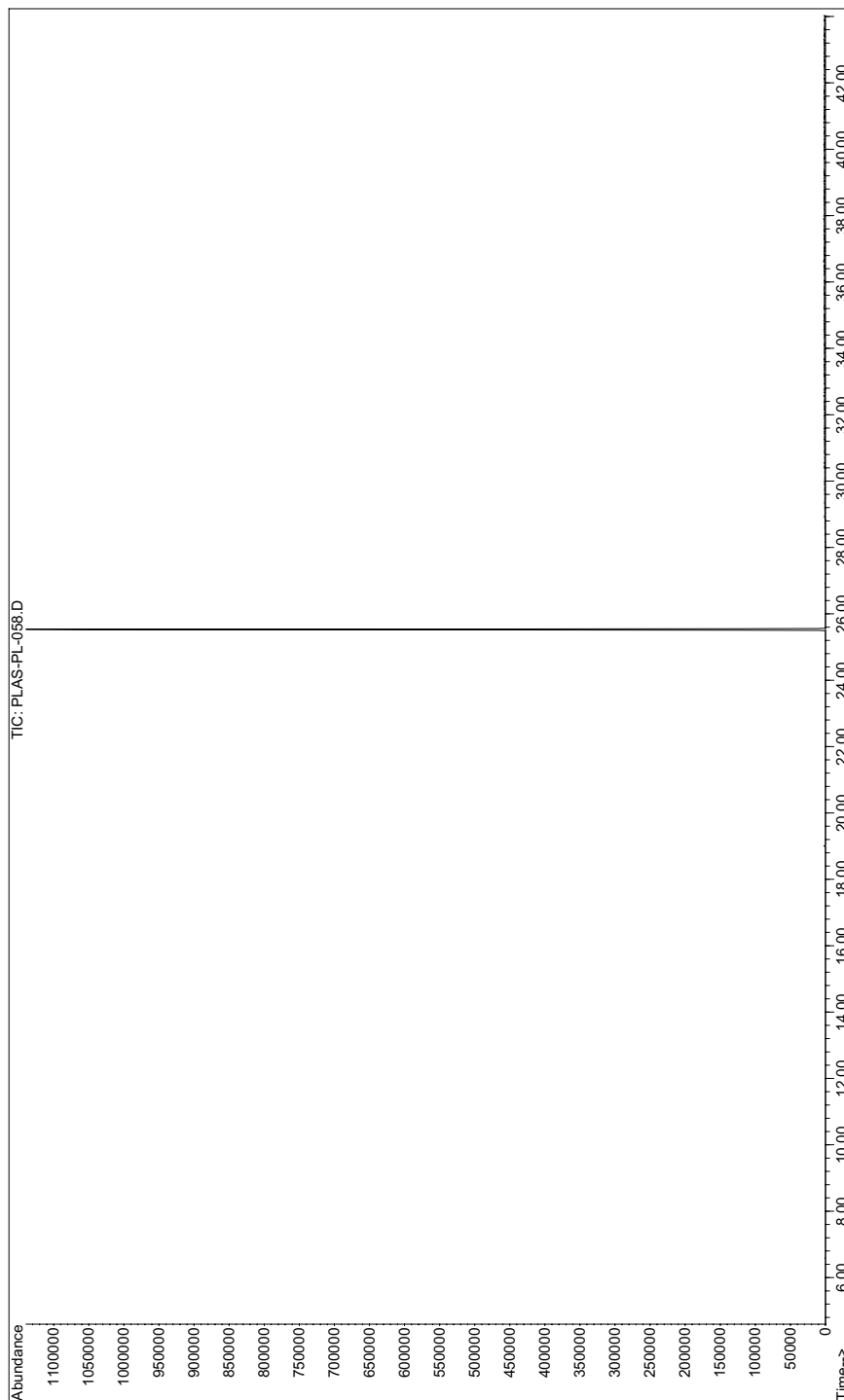
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Witamol 500 - PLAS-PL-058*

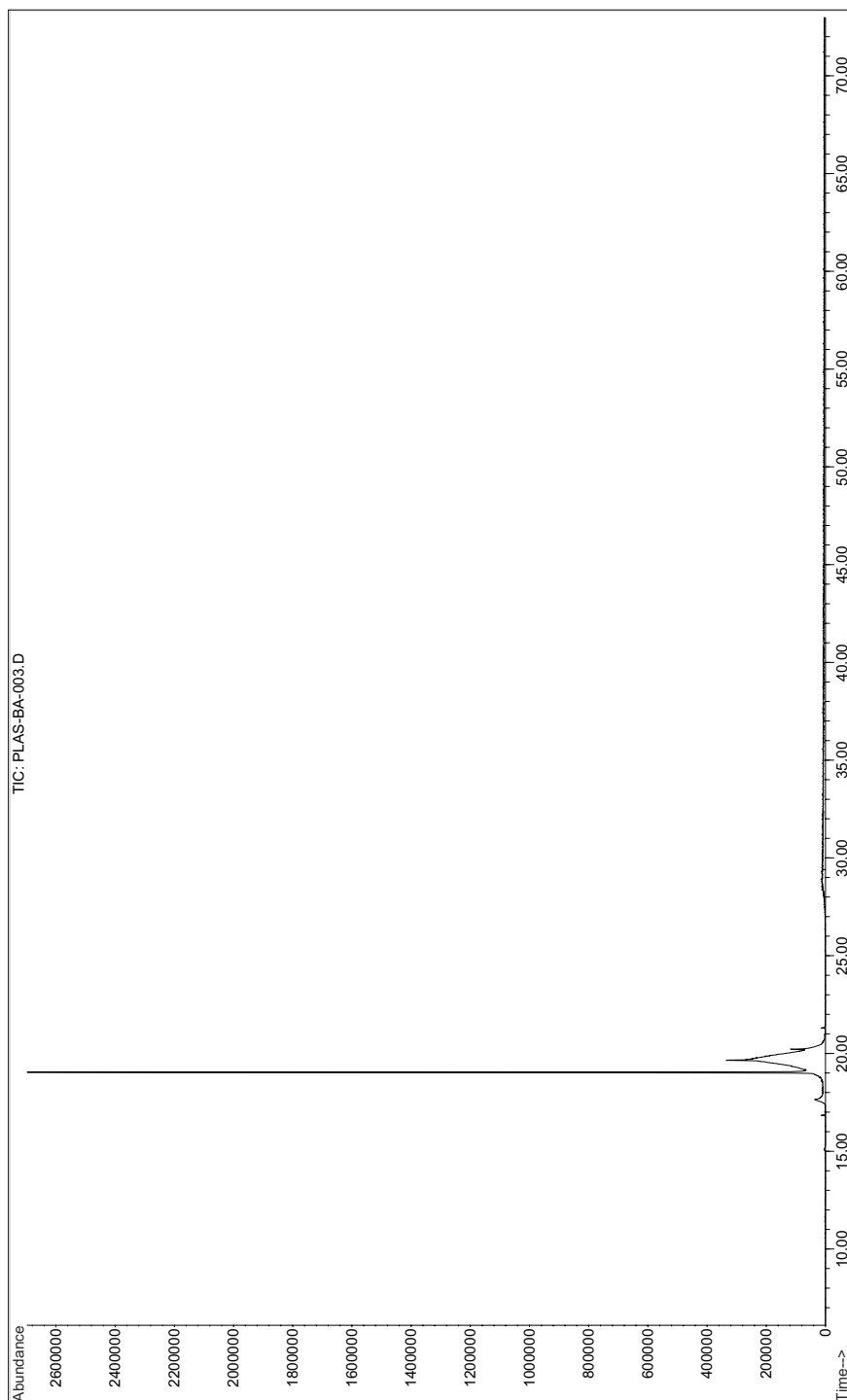
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

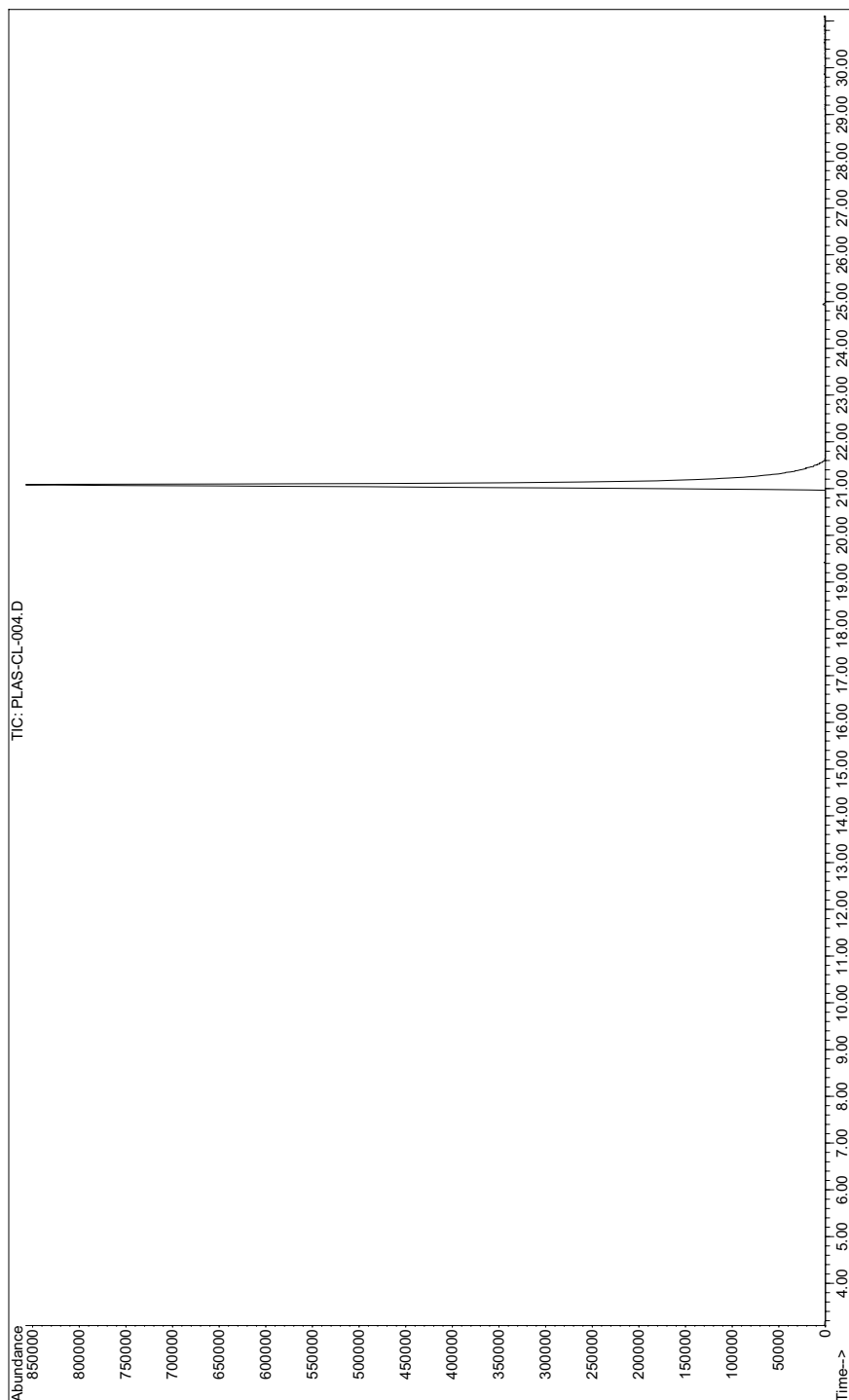
Chromatogram for *Celogen® RA - PLAS-BA-003*

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



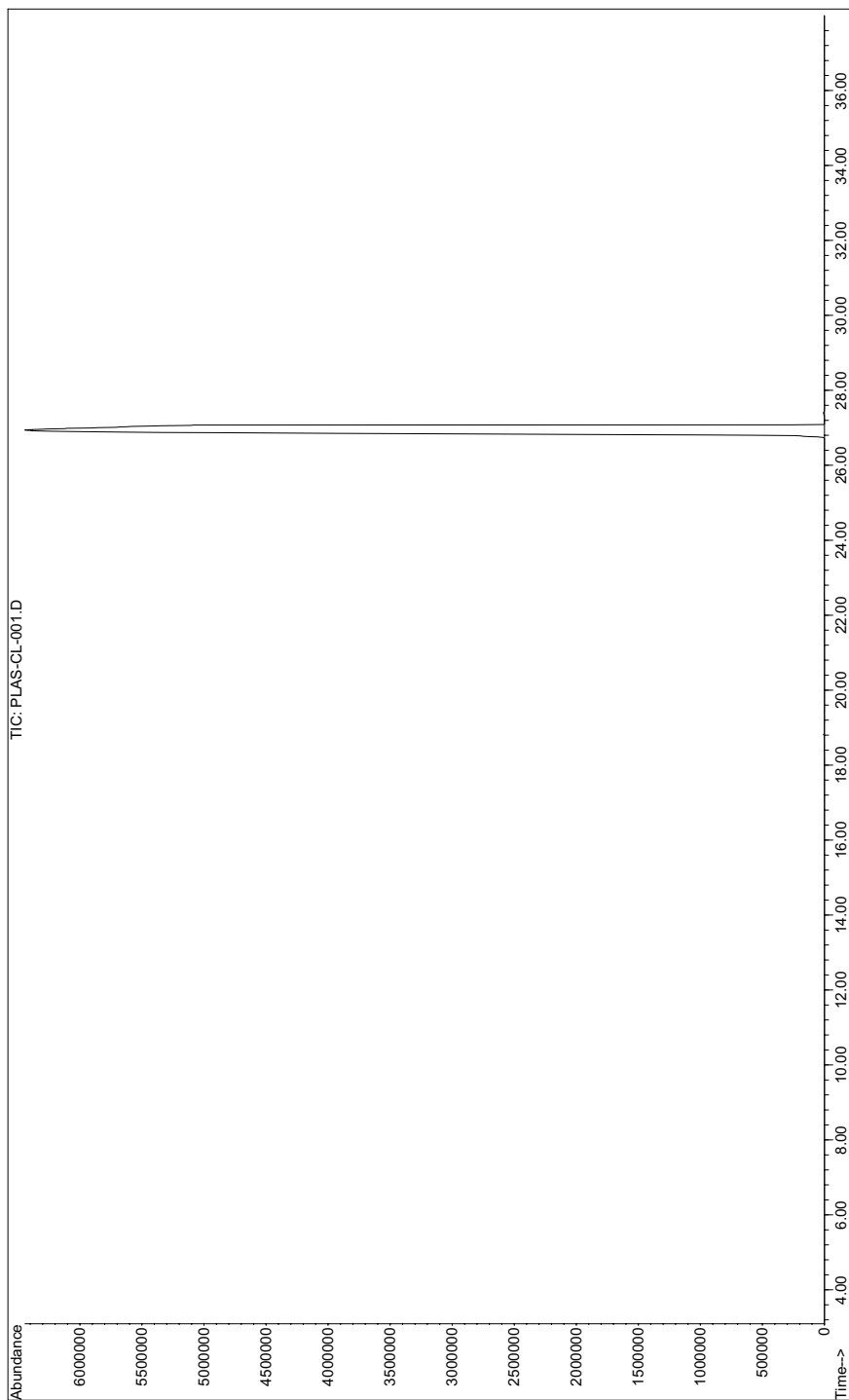
*Analytical Information***Chromatogram for *Perkacit*[®] DPG - PLAS-CL-004****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

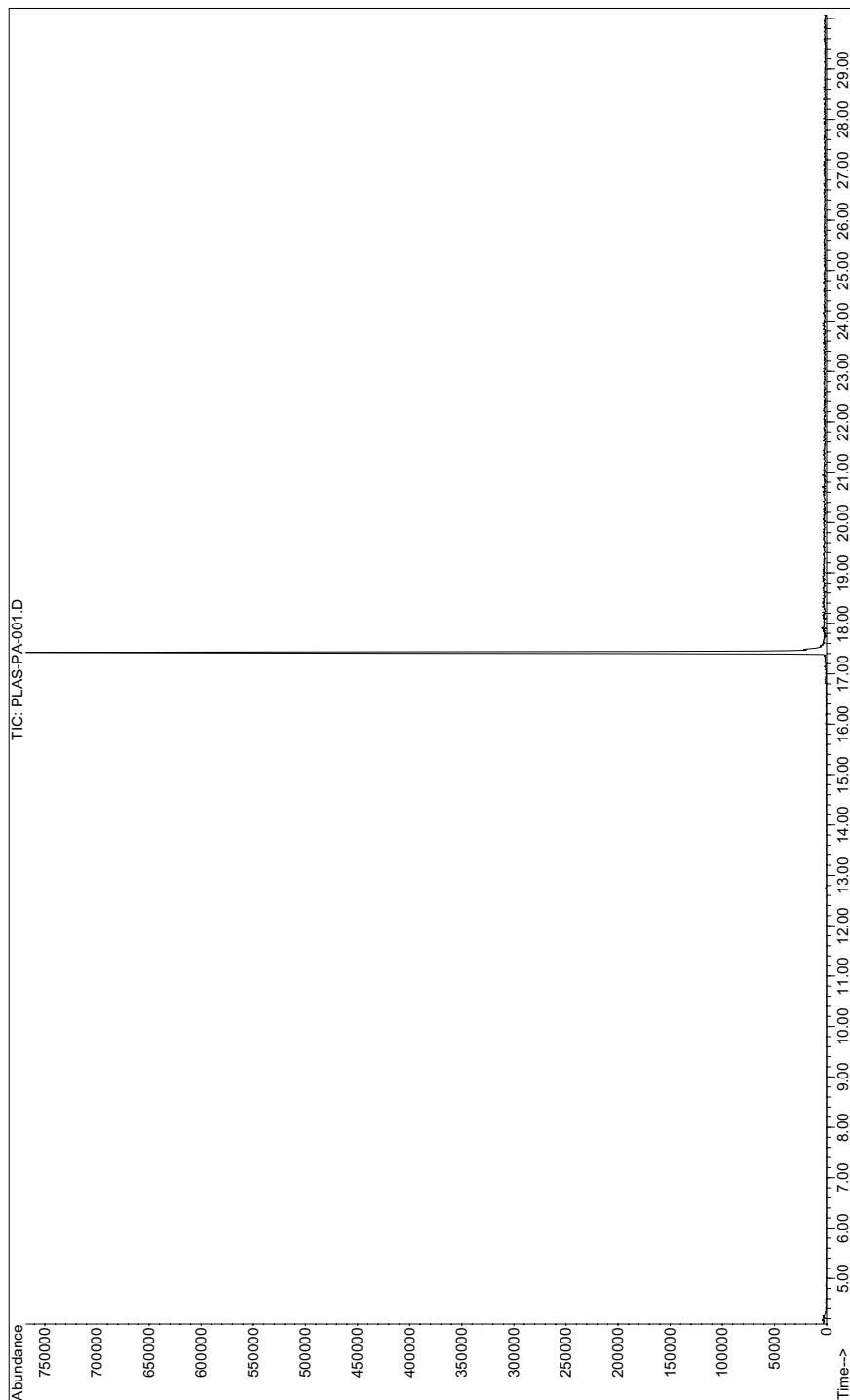
Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for *Perkacit*[®] MBTS - PLAS-CL-001****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

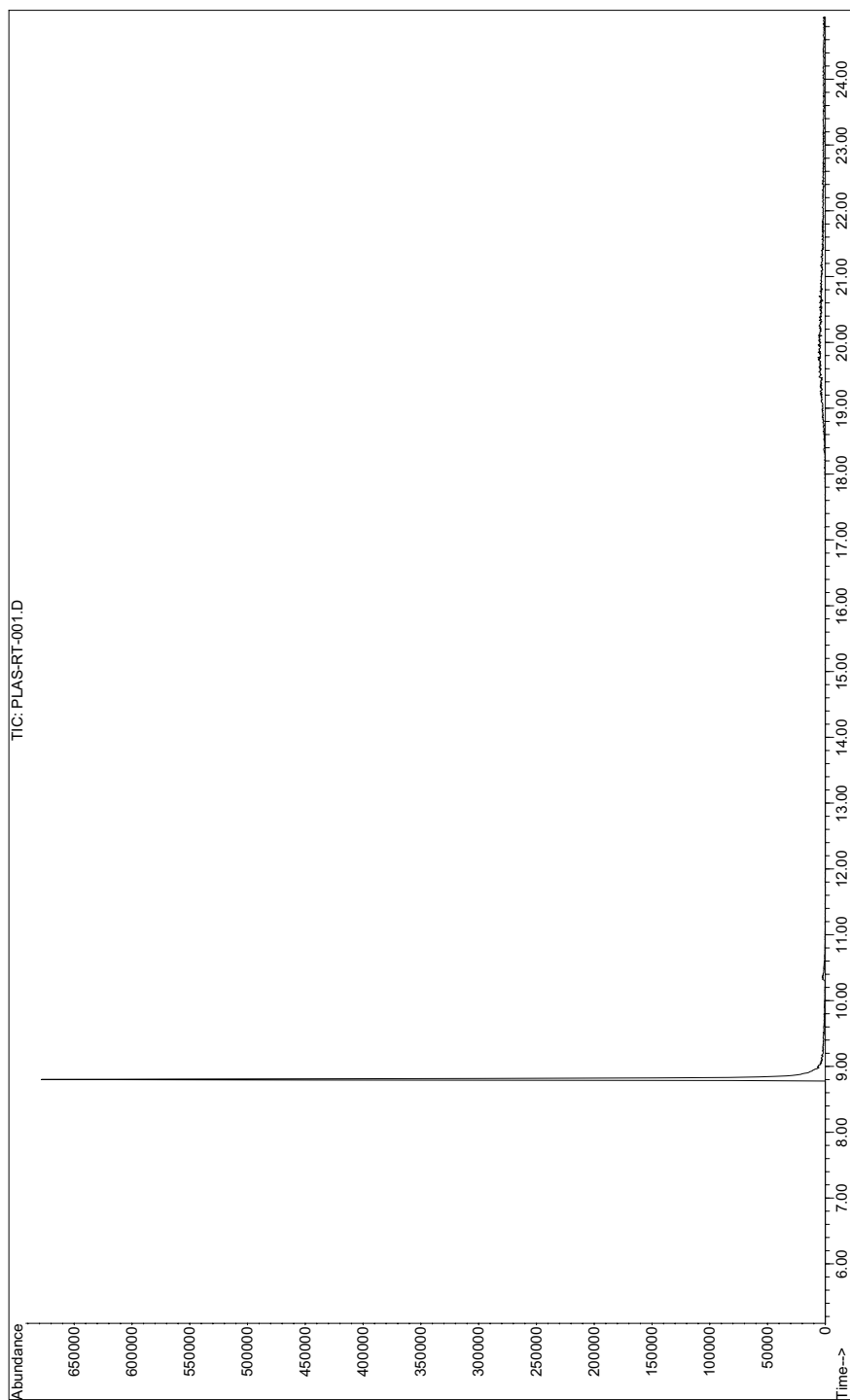
Inj Temp=250 °C, Det=MSD

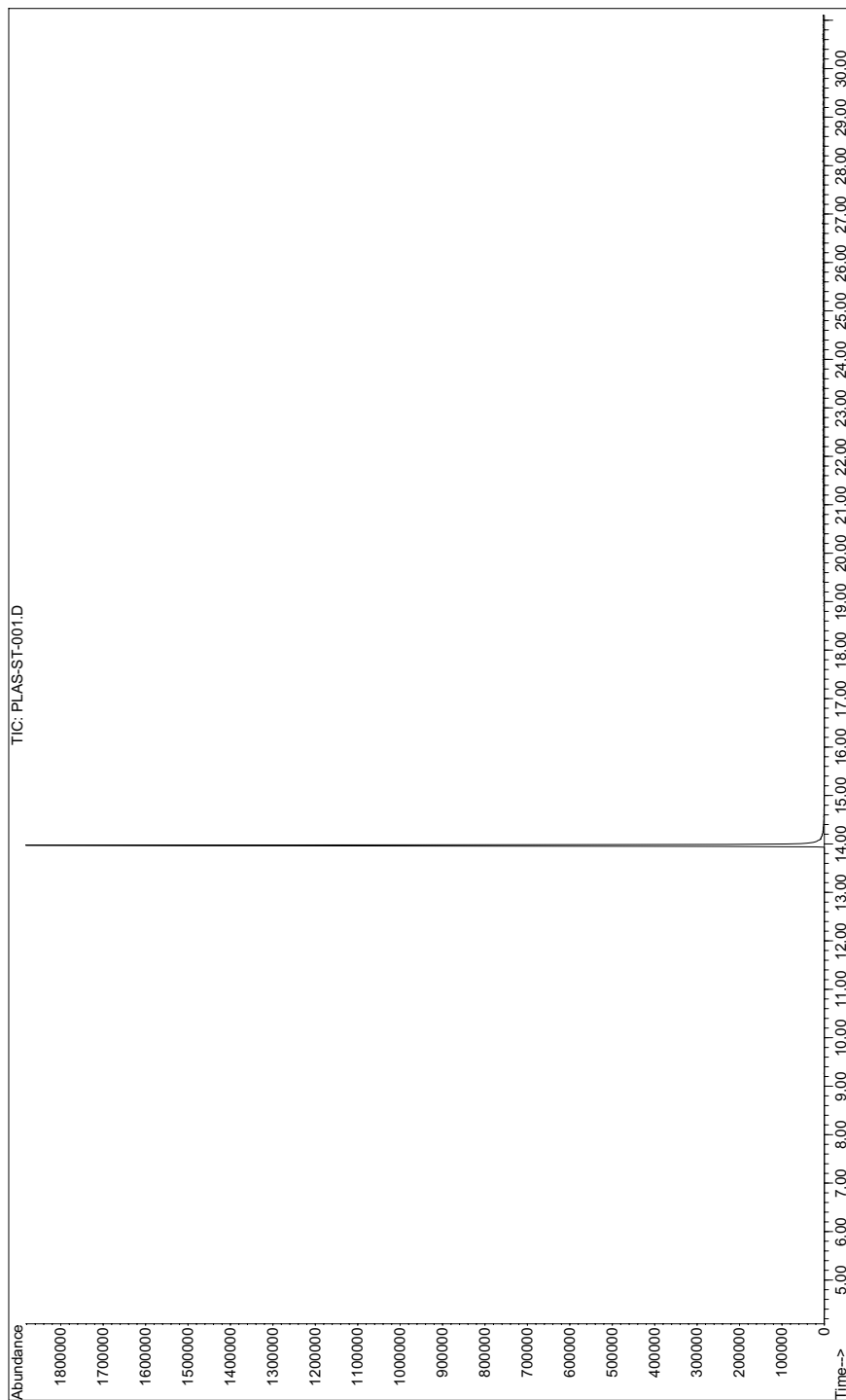


*Analytical Information***Chromatogram for *Kemamide*[®] *E ultra* - PLAS-PA-001****Analytical Conditions Summary** 50 °C (0 min) to 350 °C (40 min) @ 15 °C/min Det=MSD

*Analytical Information***Chromatogram for Retarder AK - PLAS-RT-001****Analytical Conditions Summary** 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min

Inj Temp=250 °C, Det=MSD



*Analytical Information***Chromatogram for Stearic Acid RG (rubber grade) - PLAS-ST-001****Analytical Conditions Summary** 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD

Definitions and Abbreviations

ABS	Acrylonitrile butadiene styrene
ACGIH	American Conference of Governmental Industrial Hygienists
ADI	Allowable daily intake
BCF	Bioconcentration Factor. The concentration of a chemical in a tissue per concentration of the chemical in water (reported as L/kg). BCF>1000 is considered a high potential for bioconcentration, between 1000 and 250 is considered moderate, and <250 is considered low. <i>See also</i> Pow.

BCF is related to Pow by the following equation:

$$\log(BCF) = 0.79\log(Pow) - 0.4$$

BR	Polybutadiene rubber
BW	Body weight
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CFR	Code of Federal Regulations
CPE	Chlorinated polyethylene
CR	Neoprene
DMP	Dimethyl phthalate
CSM	Chlorosulfonated polyethylene
CWA	Clean Water Act
DMP	Dimethyl phthalate
DOT	Department of Transportation
E	Emulsifiable (as used in the solubility section)
ENR	Epoxidized natural rubber
EPM	Ethylene propylene rubber. <i>See also</i> EPDM.
EPDM	Ethylene propylene rubber. <i>See also</i> EPM.
EVA	Ethylene vinyl acetate
FDA	Food and Drug Administration (US). www.fda.gov
GRAS	Generally regarded as safe
HDPE	High density polyethylene
HRGC	High resolution gas chromatography
HRMS	High resolution mass spectrometry
IARC	International Agency for Research on Cancer
LC50	Lethal Concentration, 50% (median lethal concentration)
LD50	Lethal Dose, 50% (median lethal dose)
LDPE	Low density polyethylene

NBR	Nitrile-butadiene rubber
NIOSH	National Institute for Occupational Safety and Health
NOAEL	No observed adverse effect level
NOEL	No observed effect level
NTP	National Toxicology Program
NR	Natural rubber
OECD	Organization for Economic Cooperation and Development. www.oecd.org
OSHA	Occupational Safety and Health Administration
PBDE	Polybrominated diphenyl ether
PCP	Polychloroprene
PE	Polyethylene
PET	Polyethylene terephthalate
PETG	Polyethylene terephthalate glycol
PMMA	Poly(methyl methacrylate)
Polyols	A collective term for polyester, polyether, and aliphatic-multifunctional alcohols. All polyols have more than one multifunctional alcohol group.
POM	Polyoxymethylene
POP	Persistent organic pollutant
Pow/Kow	log Pow or Kow are the partition coefficients of n-octanol/water. Substances with log Pow >3 are typically judged to have the potential to bioaccumulate. <i>See also</i> BCF.
PP	Polypropylene
PS	Polystyrene
PVC	Polyvinyl chloride
RTECS	Registry of Toxic Effects of Chemical Substance
SBR	Styrene-butadiene rubber
SIS	Styrene-isoprene-styrene
TDLo	Lowest Published Toxic Dose
TPV	Thermoplastic vulcanizate
TSCA	Toxic Substances Control Act
U	Unknown (as used in the solubility section)
UR	Butyl rubber
UV	Ultraviolet

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102.11	32	315.80	100	447.57	88
132.24	228	318.32	264	454.56	376
132.23	44	323.43	82	462.62	350
148.12	400	326.28	382	464.01	336
164.23	80	326.43	64	467.45	186
167.25	30	330.46	344	474.72	332
173.25	200	332.48	396	480.72	212
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182.15	246	336.38	346	530.87	136
188.33	120	337.58	398	514.70	268
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206.32	104	340.31	270	530.92	330
211.27	394	340.50	294	530.93	352
212.20	210	340.55	110	538.94	222
213.28	118	342.39	366	546.78	306
214.22	62	351.49	146	552.79	158
216.32	380	354.52	342	564.69	234
218.20	334	354.57	254	564.72	233
219.28	188	356.44	124	600-700	58
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225.27	70	361.93	42	638.92	152
228.31	46	362.40	372	642.93	148
229.26	392	362.50	320	643.59	236
230.30	292	368.37	316	643.62	235
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236.38	226	370.57	248, 348	683.30	116
238.38	34	377.52	172	689.00	76
239.32	50	382.58	102	689.32	190
250.38	166	384.70	48	697	208
258.35	370	390.56	288, 296, 304, 360	699.92	106
260.36	184			722.48	237
262.43	160	398.63	284	733.03	126
263.42	140	402.54	266	775.32	132
264.41	36	405.57	170	784.08	154
266.31	378	408.76	38	852.97	122
268.40	54	412.65	356	959.22	238
274.29	68	418.61	326	971.22	245
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55	60	73	129	284	284.48	100	98	87	32	26	Stearic Acid, 409
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55	74	125	98	199	230.30	100	74	125	98	199	Dimethyl sebacate, 263
55	97	166	84	240	354.57	100	35	31	31	5	Butyl ricinoleate, 315
57	69	83	155	97	424.74	100	32	16	15	14	Flexol EP-8, 279
57	69	84	113	155	424.74	100	27	17	14	10	Flexol EP-8, 281
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57	71	83	155	295	1037.39	100	59	26	19	2	Epoxidized linseed oil, 271
57	71	83	155	297	1037.39	100	49	26	20	2	Epoxidized linseed oil, 269
57	71	84	155	353	1037.39	100	57	27	17	1	Epoxidized linseed oil, 270
57	86	76	55	56	408.76	100	77	72	40	23	Cure-Rite [®] IBT, 39
57	117	71	100	229	340.50	100	63	54	37	2	Diocetyl maleate, 265
57	261	303	275	332	332.57	100	92	37	32	9	Isonox [®] 232, 161
233	217	204	234	438	438.69	100	40	22	18	14	Ethaphos [®] 368, 143
57	441	442	147	646	646.92	100	56	17	15	7	Ethaphos [®] 368, 141
57	604	117	287	279	604	100	56	45	36	31	Alkanox [®] P27, 67
59	55	72	43	337	337.58	100	60	51	48	3	Kemamide [®] E ultra, 405
70	134				733.03	100	16				O,O'-Dioctadecylpentaerythritol bis(phosphite), 121

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71	89	56	55	53	216.32	100	79	71	22	20		2,2,4-Trimethyl-1,3-pentanediol-isobutyrate, 387
71	315	213	129	514	514.708	100	65	60	27	1		Citroflex [®] B-6, 329
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76	104	50	74	148	148.12	100	99	63	24	16		Retarder AK, 407
81	55	67	95	96	354.52	100	97	97	78	73		Methyl O-Acetylricinoleate, 349
91	71	149	132	238	454.56	100	31	28	17	13		Santicizer [®] 278, 211
91	106	92	65	213	213.28	100	45	19	15	5		Dibenzylhydroxylamine, 111
93	77	211	51	65	211.27	100	44	21	19	15		Perkacit [®] DPG, 401
94	346				733.03	100	19					O,O'-Diocetadecylpentaerythritol bis(phosphite), 122
98	167	168	108	264	264.41	100	78	17	16	7		Accelerator CBTS, 37
99	155	127	81	182	182.15	100	91	56	49	5		Triethylphosphate, 385
99	155	211	57	125	266.31	100	25	16	9	9		Tributylphosphate, 383
101	129	55	73	174	174.19	100	59	26	19	1		Diethyl succinate, 253
102	45	73	42	59	102.16	100	21	20	20	7		Accelerator ETU-22 PM, 33
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105	149	77	45	89	420.14	100	40	38	25	17		Hercoflex [®] 900, 283
105	149	77	51	106	342.39	100	80	55	15	8		Polycizer [®] DP 500, 375
105	149	77	51	179	314.33	100	95	51	14	1		Benzoflex [®] 2-45, 311
105	149	77			420.14	100	70	33				Hercoflex [®] 900, 285
105	163	77	106	51	342.39	100	48	31	8	4		Polycizer [®] DP 500, 373
105	163	77	51	106	342.39	100	66	39	8	8		Polycizer [®] DP 500, 374
188	72	57	90	155	188.33	100	50	43	34	26		N,N'-Dibutylthiourea, 113
111	55	157	128	202	202.25	100	96	85	69	1		Diethyl adipate, 339
114	59	55	111	102	174.19	100	94	83	74	65		Dimethyl adipate, 261
116	360	88	362	60	361.93	100	68	55	51	44		Accelerator EZ & EZ-SP, 43
117	75	87	105	132	132.24	100	32	29	21	1		Silquest [®] A-2171, 231
121	107	163	177	220	689.00	100	54	36	15	7		Naugard [®] RM, 203

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124	58	125	140	107	480.72	100	11	9	8	3	Bis(2,6,6-tetramethyl-4-piperid) sebacate, 213
124	460	58	321	599	599.09	100	57	50	37	12	BLS 1944, 79
124	98	58	141	140	599.09	100	96	66	29	24	BLS 1944, 79
129	112	83	147	370	370.57	100	29	25	18	1	Morflex [®] 310, 355
129	241	55	111	370	370.57	100	66	58	34	1	Adimoll DO, 309
129	255	85	111	398	398.62	100	58	34	25	1	Diisononyl adipate, 256
129	255	85	111	398	398.62	100	63	33	26	1	Diisononyl adipate, 255
129	255	85	111	398	398.62	100	65	34	27	1	Diisononyl adipate, 257
129	269	111	287	426	426.67	100	70	29	10	1	Polycizer [®] 632, 369
132	60	71	131	133	132.23	100	38	19	15	8	N, N'-Diethylthiourea, 119
135	77	51	50	136	228.31	100	55	22	12	9	1,3-Diphenyl-2-thiourea, 127
135	107	91	220	77	689.00	100	15	5	4	4	Naugard [®] RM, 204
135	107	136	121	91	689.32	100	18	10	7	6	Naugard [®] PHR, 189
135	107	136	91	77	689.32	100	20	10	7	6	Naugard [®] PHR, 191
135	107	149	121	55	689.32	100	78	63	48	19	Alkanox [®] TNPP, 69
135	107	149	121	191	689.32	100	92	78	57	22	Naugard [®] PHR, 190
135	121	107	149	220	689.00	100	40	36	33	8	Naugard [®] RM, 205
138	72	139	56	154	508.78	100	10	10	6	3	BLS 292, 83
170	70	102	186	85	283	100	61	56	44	32	BLS 292, 83
139	91	123	278	155	229.26	100	62	38	36	24	Celogen [®] RA, 399
148	57	279	71	14	390.56	100	21	17	16	10	Diisooctyl phthalate, 259
149	57	55	150	265	N/A	100	12	10	10	5	Celogen [®] SD-125, 317
149	57	55	150	56	N/A	100	13	11	10	6	Celogen [®] SD-125, 318
149	57	55	150	69	N/A	100	12	11	10	6	Celogen [®] SD-125, 319
149	57	71	293	418	418.61	100	39	30	24	1	Jayflex [®] DINP, 301
149	57	71	293	418	418.61	100	39	32	26	1	Jayflex [®] DINP, 299
149	57	71	293	418	418.61	100	41	34	25	1	Jayflex [®] DINP, 300
149	57	71	307	446	446.66	100	40	28	27	1	Jayflex [®] DIDP, 297
149	57	265	104	76	362.50	100	13	12	5	3	Jayflex [®] 77, 295

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149	57	265	99	104	362.50	100	21	16	8	6	Jayflex [®] , 294
149	57	349	335	531	530.93	100	39	34	11	1	Morflex [®] x-1125, 359
149	57	349	355	530	530.92	100	58	34	7	1	Jayflex [®] DTD, 303
149	91	206	123	132	312.37	100	65	27	13	13	Santicizer [®] 160, 381
149	104	150	223	278	278.34	100	11	10	4	1	Dibutyl Phthalate, 335
149	121	164	91	77	600-700	100	72	35	19	17	Lowinox [®] CPL, 51
149	167	104	279	390	390.56	100	30	11	10	1	Diethyl Phthalate, 267
149	167	55	249	83	330.46	100	32	14	7	6	Morflex [®] 150, 351
149	177	104	121	222	222.24	100	19	13	8	1	Diethyl Phthalate, 251
149	193	66	70		420.14	100	62	12	10		Hercoflex [®] 900, 284
149	263	77	133	57	336.38	100	37	16	14	12	Morflex [®] 190, 353
149	279	104	261	390	390.56	100	12	4	2	1	Polycizer [®] 162, 367
149	321	150	57	474	474.72	100	11	11	8	1	Jayflex [®] L11P-E Plasticizer, 305
151	257	274	124	108	274.29	100	30	29	15	12	Uvinul [®] 3049, 61
153	170	212	79	51	212.20	100	80	25	11	8	Propyl gallate, 209
157	115	203	111	277	276.32	100	35	17	9	1	Citroflex [®] 2, 321
157	203	115	213	273	318.32	100	42	21	12		Citroflex [®] A-2, 325
158	159	115	157	173	173.25	100	12	8	7	5	Naugard [®] Q Extra, 199
161	203	129	218	175	784.08	100	77	52	51	44	Irganox [®] 3114 FF, 153
163	77	50	92	194	194.19	100	19	11	11	6	Hi-Point [®] PD-1, 287
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163	134	175	119	221	221.37	100	66	46	44	1	Silquest [®] A-1100, 223
163	135	178	91	77	699.92	100	47	35	16	13	Cyanox [®] 1790, 99
163	199	79	63	276	276.55	100	23	23	9	7	Silquest [®] A-137, 227
164	163	106	77	51	164.23	100	65	32	12	10	Antioxidant 60, 73
167	69	108	63	123	167.25	100	23	15	15	11	Accelerator MBT, MBT/MG, 31
169	168	167	51	83	N/A	100	67	35	16	13	Naugard [®] A, 175
170	70	102	186	85	283	100	61	56	44	32	BLS 1622, 77
170	300	70	168	284	283	100	58	47	31	13	BLS 1622, 77
171	55	255	152	83	356.54	100	86	78	41	31	Plastolein 9050, 365

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175	190	58	235	176	699.92	100	77	63	20	15	Cyanox [®] 1790, 100
177	161	149	57	340	340.55	100	75	51	44	39	Cyanox [®] 2246, 103
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185	57	70	71	112	426.67	100	33	24	22	21	2-Ethylhexyl sebacate, 273
185	129	55	111	258	258.35	100	95	84	71	1	Polycizer [®] W 260, 377
185	129	57	259	351	276.32	100	73	27	25	1	Citroflex [®] 4, 323
185	129	259	57	403	402.54	100	56	52	26	1	Citroflex [®] A-4, 327
191	57	192	206	91	604	100	21	15	15	7	Alkanox [®] P27, 67
191	175	163	57	368	368.55	100	68	56	46	39	Cyanox [®] 425, 105
191	206	57	91	419	604.69	100	16	11	5	1	Ultranox [®] 626, 219
191	206	131	163	57	206.32	100	21	15	14	13	2,6-Di-tert-butylphenol, 97
191	206	192	131	115	N/A	100	24	15	10	8	BNX 1225 TPR, 87
193	149	104	50	475	~800	100	39	35	8	1	Paraplex [®] G-30, 361
193	208	91	77	73	699.92	100	36	19	16	13	Cyanox [®] 1790, 101
194	193	195	192	209	N/A	100	21	21	11	11	Naugard [®] A, 175
205	220	57	206	145	600-700	100	24	16	16	12	Lowinox [®] CPL, 52
205	220	57	145	177	220.35	100	42	20	18	14	Naugard [®] BHT, 179
211	268	183	167	253	362.50	100	49	19	14	11	Jayflex [®] 77, 293
211	268	183	105	253	268.40	100	46	16	15	10	Santoflex [®] 6PPD, 47
213	137	214	77	51	214.22	100	80	67	46	30	Uvinul [®] 3000, 55
213	228	119	91	65	228.29	100	22	16	10	7	Bisphenol A, 313
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219	57	232	203	552	552.79	100	88	63	47	46	Irganox [®] MD 1024, 157
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219	191	234	57	220	775.32	100	27	26	18	16	Ethanox [®] 330, 132
219	218	217	108	115	219.28	100	64	51	23	16	Naugard [®] PANA, 187
219	234	220	57	91	234.38	100	23	17	10	6	2,6-Di-tert-butyl-4-ethylphenol, 91

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219	263	58	163	203	263.42	100	26	19	12	12	Ethanox [®] 703, 139
219	341	356	203	147	356.44	100	83	72	58	56	Diethyl 3,5-Di-tert-butyl-4-hydroxybenzylphosphonate, 117
315	91	316	330	103	356.44	100	46	30	30	27	Diethyl 3,5-Di-tert-butyl-4-hydroxybenzylphosphonate, 117
221	250	222	192	71	250.38	100	19	16	10	8	Lowinox [®] AH25, 165
225	93	65	168	154	225.27	100	20	12	10	18	Tinuvin [®] PED, 63
226	225	165	227	152	N/A	100	45	28	16	10	Vinsol [®] resin, 391
227	151	228	77	51	228.26	100	81	66	38	21	Uvinul [®] 3040, 59
232	301	141	797	959	959.22	100	61	60	22	9	Decabromodiphenyl ether, 240
233	247	234	262	57	N/A	100	28	18	17	15	Naugard [®] PS-35, 197
233	247	262	57	217	262.43	100	29	17	10	6	Isonox [®] 132, 159
233	248	234	205		775.32	100	24	17	16		Ethanox [®] 330, 133
233	304	234	43	107	304.58	100	39	17	16	15	Santoflex [®] 77PD, 49
240	239	165	241	152	N/A	100	45	26	18	13	Vinsol [®] resin, 391
241	185	55	56	57	314.46	100	72	31	29	24	Dibutyl Sebacate, 337
247	57	261	248	332	332.57	100	32	25	19	4	Isonox [®] 232, 162
247	261	57	55	332	332.57	100	64	63	23	5	Isonox [®] 232, 163
251	250	94	249	252	362.40	100	24	18	16	13	Santicizer [®] 141, 378, 379
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266	98	194	123	85	~255	100	31	28	24	19	Halowax 1001, 245
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266	267	337	250	393	N/A	100	21	14	10	1	Naugard [®] PS-35, 197
266	281	267	97	125	N/A	100	32	21	15	7	Naugard [®] PS-30, 193
277	57	292	147	219	1177.65	100	41	37	28	23	Naugard [®] B-25, 177
277	147	292	57	219	460.73	100	44	32	23	10	BNX 1077, 85
277	193	278	379	462	462.62	100	22	17	8	1	Morflex [®] 560, 357
277	292	147	219	57	642.93	100	39	24	22	21	Irganox [®] 1035, 147
277	292	147	57	219	1177.65	100	38	32	26	22	Ethanox [®] 310, 129

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277	292	219	278	203	N/A	100	38	22	19	13	BNX 1225 TPR, 88
285	1537				733.03	100	15				O,O'-Diocetadecylpentaerythritol bis(phosphite), 123
292	289	293	220	222	N/A	100	84	49	49	26	Aroclor 1242, 241
300	242	108	122	166	332.48	100	56	37	16	12	Perkacit [®] MBTS, 403
305	193	57	306	323	56.78	100	27	23	20	16	Tris(2-ethylhexyl) Trimellitate, 277
315	330	316	91	237	852.97	100	34	26	22	16	3,9-Bis(2,4-dicumylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro(5.5)undecane, 115
322	323	250	393	57	N/A	100	27	17	14	6	Naugard [®] PS-30, 195
326	325	77	65	170	340.31	100	82	47	27	23	Cresyl Diphenyl Phosphate, 331
326	325	77	65	215	326.28	100	84	48	28	24	Triphenylphosphate, 389
326	325	169	215	94	368.37	100	88	25	23	20	Imol S-140, 289
331	332	158	346	315	173.25	100	27	18	6	6	Naugard [®] Q Extra, 200
339	340	32	148	41	382.58	100	27	8	6	4	4,4'-Butylidenebis(6-tert-butyl-m-cresol), 95
340	339	77	165	341	340.31	100	70	34	21	20	Cresyl Diphenyl Phosphate, 332
354	165	104	181	368	368.37	100	32	16	13	1	Imol S-140, 290
354	353	165	77	91	340.31	100	60	34	33	26	Cresyl Diphenyl Phosphate, 333
358	164	149	136	302	358.54	100	98	84	26	7	Irganox [®] 1081, 149
358	343	359	136	164	358.54	100	41	25	21	13	Lowinox [®] TBM-6, 167
360	362	290	325	218	N/A	100	76	63	24	20	Aroclor 1254, 242
362	377	363	378	105	377.52	100	81	29	24	15	Naugard [®] 635, 171
362	377	363	378	105	377.52	100	85	30	26	23	Naugard [®] 635, 172
362	377	363	378	165	377.52	100	66	29	20	17	Naugard [®] 635, 173
371	372	355	170	178	173.25	100	29	22	20	15	Naugard [®] Q Extra, 201
382	91	165	103	179	368.37	100	31	30	29	24	Imol S-140, 291
384	140	152	283	218	384.70	100	94	91	81	80	Dipentamethylenethiuram Tetrasulfide, 125
390	405	391	406	187	405.57	100	54	31	18	15	Naugard [®] 445, 169
390	405	391	406	187	531/406	100	56	31	18	16	Naugard [®] HM-22, 181
404	332	262	120	166	403.73	100	49	23	21	17	Halowax 1051, 246
406	404	465	563	297	564.72	100	99	90	89	20	2,2',4,4',5-Pentabromodiphenyl ether, 235

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409	424	367	57	219	424.66	100	80	28	25	14	Ethanox [®] 702, 137
415	430	105	200	416	430.56	100	92	37	30	28	2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole), 215
430	165	205	57	121	430.71	100	71	8	6	4	Irganox [®] E 201, 155
430	428	432	358	288	N/A	100	94	65	63	30	Aroclor 1260, 243
432	91	119	447	103	447.57	100	92	66	57	43	BLS 234, 81
441	57	442	147	308	N/A	100	58	32	24	10	BNX 1225 TPR, 89
441	57	442	147	646	646.92	100	82	31	23	12	Naugard [®] B-25, 177
460	57	177	215	445	600-700	100	78	38	38	32	Lowinox [®] CPL, 53
466	57	468	116	467	467.45	100	60	57	29	26	Naugard [®] NBC, 185
466	57	468	467	116	467.45	100	64	53	28	24	Naugard [®] NBC, 185
484	74	486	482	62	643.62	100	87	72	62	49	2,2',4,4',5,5'-Hexabromodiphenyl ether, 237
484	486	488	482	971	971.22	100	97	60	42	5	Saytex 8010, 247
484	643	74	486	645	643.59	100	93	82	72	72	2,2',4,4',5,6'-Hexabromodiphenyl ether, 238
486	326	487	483	63	485.82	100	86	68	67	57	2,2',4,4'-Tetrabromodiphenyl ether, 234
529	527	531	544	293	543.91	100	69	68	25	18	Firemaster BP4A, 244
530	57	515	219	531	531/406	100	56	41	37	37	Naugard [®] HM-22, 181
530	57	515	531	219	530.87	100	66	44	39	33	Ethanox [®] 376, 135
563	561	723	74	721	722.48	100	99	69	68	66	2,2',3,4,4',5',6'-Heptabromodiphenyl ether, 239
565	563	406	404	137	564.69	100	98	76	74	25	2,2',4,4',6-Pentabromodiphenyl ether, 236
603	91	57	617	469	689.32	100	68	58	50	48	Alkonox [®] TNPP, 70
603	469	617	57	631	689.32	100	67	62	40	39	Alkanox [®] TNPP, 71
44	60	43	42	41	60.07	100	65	25	9	3	Activator OT Urea, 41
45	57	71	166	243	~400	100	78	49	10	1	Markstat [®] 51, 339
45	89	57	71	279	~400	100	67	48	31	6	Markstat [®] 51, 340
45	89	133	177	356	~400	100	72	36	10	1	Markstat [®] 51, 341
55	57	71	143	69	683.30	100	88	36	34	33	Cyanox [®] STDP, 117
55	57	143	69	71	514.85	100	76	29	28	28	Cyanox [®] LTDP, 115
55	60	73	129	284	284.48	100	98	87	32	26	Stearic Acid, 403
55	69	265	83	97	338.57	100	70	63	61	5	Polycizer [®] Butyl Oleate, 365
55	74	125	98	199	230.30	100	74	125	98	199	Dimethyl sebacate, 293

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55	97	166	84	240	354.57	100	35	31	31	5	Butyl ricinoleate, 255
57	69	83	155	97	424.74	100	32	16	15	14	Flexol EP-8, 309
57	69	84	113	155	424.74	100	27	17	14	10	Flexol EP-8, 311
57	69	84	155	112	424.74	100	45	31	19	13	Flexol EP-8, 310
57	71	83	155	295	1037.39	100	59	26	19	2	Epoxidized linseed oil, 301
57	71	83	155	297	1037.39	100	49	26	20	2	Epoxidized linseed oil, 299
57	71	84	155	353	1037.39	100	57	27	17	1	Epoxidized linseed oil, 300
57	86	76	55	56	408.76	100	77	72	40	23	Cure-Rite® IBT, 39
57	117	71	100	229	340.50	100	63	54	37	2	Dioctyl maleate, 295
57	261	303	275	332	332.57	100	92	37	32	9	Isonox® 232, 163
57	441	442	147	646	646.92	100	56	17	15	7	Ethaphos® 368, 143
57	604	117	287	279	604	100	56	45	36	31	Alkanox® P27, 75
59	55	72	43	337	337.58	100	60	51	48	3	Kemamide® E ultra, 399
70	134				733.03	100	16				O,O'-Diocetadecylpentaerythritol bis(phosphite), 127
71	83	56	98	55	216.32	100	45	31	28	26	2,2,4-Trimethyl-1,3-pentanediol-isobutyrate, 381
71	89	56	55	53	216.32	100	79	71	22	20	2,2,4-Trimethyl-1,3-pentanediol-isobutyrate, 381
71	315	213	129	514	514.708	100	65	60	27	1	Citroflex® B-6, 269
73	60	55	57	129	464.01	100	91	75	43	31	Laurex®, 337
76	104	50	74	148	148.12	100	99	63	24	16	Retarder AK, 401
81	55	67	95	96	354.52	100	97	97	78	73	Methyl O-Acetylricinoleate, 343
91	71	149	132	238	454.56	100	31	28	17	13	Santicizer® 278, 377
91	106	92	65	196	213.28	100	45	19	15	5	Dibenzylhydroxylamine, 119
93	77	211	51	65	211.27	100	44	21	19	15	Perkacit® DPG, 395
94	346				733.03	100	19				O,O'-Diocetadecylpentaerythritol bis(phosphite), 128
98	167	168	108	264	264.41	100	78	17	16	7	Accelerator CBTS, 37
99	155	127	81	182	182.15	100	91	56	49	5	Triethylphosphate, 246
99	155	211	57	125	266.31	100	25	16	9	9	Tributylphosphate, 379
101	129	55	73	174	174.19	100	59	26	19	1	Diethyl succinate, 283
102	45	73	42	59	102.16	100	21	20	20	7	Accelerator ETU-22 PM, 33
103	145	116	86	73	218.20	100	81	43	17	13	Kesscoflex TRA, 335

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105	149	77	45	89	420.14	100	40	38	25	17	Hercoflex [®] 900, 313
105	149	77	51	106	342.39	100	80	55	15	8	Polycizer [®] DP 500, 369
105	149	77	51	179	314.33	100	95	51	14	1	Benzoflex [®] 2-45, 251
105	149	77			420.14	100	70	33			Hercoflex [®] 900, 315
105	163	77	106	51	342.39	100	48	31	8	4	Polycizer [®] DP 500, 367
105	163	77	51	106	342.39	100	66	39	8	8	Polycizer [®] DP 500, 368
188	72	57	90	155	188.33	100	50	43	34	26	N,N'-Dibutylthiourea, 121
111	55	157	128	202	202.25	100	96	85	69	1	Diethyl adipate, 279
114	59	55	111	101	174.19	100	94	83	74	65	Dimethyl adipate, 291
116	360	88	362	60	361.93	100	68	55	51	44	Accelerator EZ & EZ-SP, 43
117	75	87	105	132	132.24	100	32	29	21	1	Silquest [®] A-2171, 229
121	107	163	177	220	689.00	100	54	36	15	7	Naugard [®] RM, 205
121	147	91	107	59	236.38	100	53	41	12	10	Silquest [®] A-187, 227
124	58	125	140	107	480.72	100	11	9	8	3	Bis(2,6,6-tetramethyl-4-piperid) sebacate, 213
124	460	58	321	599	599.09	100	57	50	37	12	BLS 1944, 87
124	98	58	141	140	599.09	100	96	66	29	24	BLS 1944, 87
129	112	83	147	370	370.57	100	29	25	18	1	Morflex [®] 310, 349
129	241	55	111	370	370.57	100	66	58	34	1	Adimoll DO, 249
129	255	85	111	398	398.62	100	58	34	25	1	Diisononyl adipate, 286
129	255	85	111	398	398.62	100	63	33	26	1	Diisononyl adipate, 285
129	255	85	111	398	398.62	100	65	34	27	1	Diisononyl adipate, 287
129	269	111	287	426	426.67	100	70	29	10	1	Polycizer [®] 632, 363
132	60	71	131	133	132.23	100	38	19	15	8	N, N'-Diethylthiourea, 45
135	77	51	50	136	228.31	100	55	22	12	9	1,3-Diphenyl-2-thiourea, 47
135	107	91	220	77	689.00	100	15	5	4	4	Naugard [®] RM, 206
135	107	136	121	91	689.32	100	18	10	7	6	Naugard [®] PHR, 191
135	107	136	91	77	689.32	100	20	10	7	6	Naugard [®] PHR, 193
135	107	149	121	55	689.32	100	78	63	48	19	Alkanox [®] TNPP, 77
135	107	149	121	191	689.32	100	92	78	57	22	Naugard [®] PHR, 192
135	121	107	149	220	689.00	100	40	36	33	8	Naugard [®] RM, 207

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138	72	139	56	154	508.78	100	10	10	6	3	BLS 292, 91
170	70	102	186	85	283	100	61	56	44	32	BLS 292, 91
139	91	278	123	155	229.26	100	56	54	42	27	Celogen [®] RA, 393
149	57	55	150	265	N/A	100	12	10	10	5	Celogen [®] SD-125, 257
149	57	55	150	56	N/A	100	13	11	10	6	Celogen [®] SD-125, 258
149	57	55	150	69	N/A	100	12	11	10	6	Celogen [®] SD-125, 259
149	57	71	293	418	418.61	100	39	30	24	1	Jayflex [®] DINP, 329
149	57	71	293	418	418.61	100	39	32	26	1	Jayflex [®] DINP, 327
149	57	71	293	418	418.61	100	41	34	25	1	Jayflex [®] DINP, 328
149	57	71	307	446	446.66	100	40	28	27	1	Jayflex [®] DIDP, 325
149	57	265	104	76	362.50	100	13	12	5	3	Jayflex [®] 77, 323
149	57	265	99	104	362.50	100	21	16	8	6	Jayflex [®] , 322
149	57	279	71	167	390.56	100	21	17	16	10	Diisooctyl phthalate, 289
149	57	349	335	531	530.93	100	39	34	11	1	Morflex [®] x-1125, 353
149	57	349	355	530	530.92	100	58	34	7	1	Jayflex [®] DTD, 331
149	91	206	123	132	312.37	100	65	27	13	13	Santicizer [®] 160, 375
149	104	150	223	278	278.34	100	11	10	4	1	Dibutyl Phthalate, 275
149	121	164	91	77	600-700	100	72	35	19	17	Lowinox [®] CPL, 59
149	167	104	279	390	390.56	100	30	11	10	1	Dioctyl Phthalate, 297
149	167	55	249	83	330.46	100	32	14	7	6	Morflex [®] 150, 345
149	177	104	121	222	222.24	100	19	13	8	1	Diethyl Phthalate, 281
149	193	66	70	237	420.14	100	62	12	10	10	Hercoflex [®] 900, 314
149	263	77	133	57	336.38	100	37	16	14	12	Morflex [®] 190, 347
149	279	104	261	390	390.56	100	12	4	2	1	Polycizer [®] 162, 361
149	321	150	57	474	474.72	100	11	11	8	1	Jayflex [®] L11P-E Plasticizer, 333
151	257	274	124	108	274.29	100	30	29	15	12	Uvinul [®] 3049, 69
153	170	212	79	51	212.20	100	80	25	11	8	Propyl gallate, 211
157	115	203	111	277	276.32	100	35	17	9	1	Citroflex [®] 2, 261
157	203	115	213	273	318.32	100	42	21	12		Citroflex [®] A-2, 265
158	159	115	157	173	173.25	100	12	8	7	5	Naugard [®] Q Extra, 201

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161	203	129	218	175	784.08	100	77	52	51	44	Irganox [®] 3114 FF, 155
163	119	79	63	276	276.55	100	23	23	9	7	Silquest [®] A-137, 225
163	119	153	197	79	538.94	100	53	48	42	38	Silquest [®] A-1289, 223
163	134	175	119	221	221.37	100	66	46	44	1	Silquest [®] A-1100, 221
163	135	178	91	77	699.92	100	47	35	16	13	Cyanox [®] 1790, 107
164	163	106	77	51	164.23	100	65	32	12	10	Antioxidant 60, 81
167	69	108	63	123	167.25	100	23	15	15	11	Accelerator MBT, MBT/MG, 31
169	168	167	51	83	N/A	100	67	35	16	13	Naugard [®] A, 177
170	70	102	186	85	283	100	61	56	44	32	BLS 1622, 85
170	300	70	168	159	283	100	58	47	31	27	BLS 1622, 85
171	55	255	152	83	356.54	100	86	78	41	31	Plastolein 9050, 359
171	71	55	112	283	412.65	100	40	33	28	6	Plasthall [®] DOZ, 357
175	190	58	235	176	699.92	100	77	63	20	15	Cyanox [®] 1790, 108
177	161	149	57	340	340.55	100	75	51	44	39	Cyanox [®] 2246, 111
177	220	135	67	149	775.32	100	52	42	41	36	Ethanox [®] 330, 133
182	223	57	238	149	238.38	100	53	52	39	35	Accelerator BBTS, 35
185	57	70	112	297	426.67	100	74	47	29	4	Witamol 500, 387
185	57	70	71	112	426.67	100	33	24	22	21	2-Ethylhexyl sebacate, 303
185	129	55	111	258	258.35	100	95	84	71	1	Polycizer [®] W 260, 371
185	129	57	259	351	276.32	100	73	27	25	1	Citroflex [®] 4, 263
185	129	259	57	401	402.54	100	56	52	26	1	Citroflex [®] A-4, 267
191	57	192	206	91	604	100	21	15	15	7	Alkanox [®] P27, 75
191	175	163	57	368	368.55	100	68	56	46	39	Cyanox [®] 425, 113
191	206	57	91	419	604.69	100	16	11	5	1	Ultranox [®] 626, 217
191	206	131	163	57	206.32	100	21	15	14	13	2,6-Di-tert-butylphenol, 105
191	206	192	163	131	N/A	100	24	15	13	10	BNX 1225 TPR, 95
193	149	104	50	475	~800	100	39	35	8	1	Paraplex [®] G-30, 355
193	208	91	77	73	699.92	100	36	19	16	13	Cyanox [®] 1790, 109
194	193	195	192	209	N/A	100	21	21	11	11	Naugard [®] A, 177
205	220	57	206	145	600-700	100	24	16	16	12	Lowinox [®] CPL, 60

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205	220	57	145	177	220.35	100	42	20	18	14	Naugard [®] BHT, 181
211	268	183	167	253	362.50	100	49	19	14	11	Jayflex [®] 77, 321
211	268	183	105	253	268.40	100	46	16	15	10	Santoflex [®] 6PPD, 55
213	137	214	77	51	214.22	100	80	67	46	30	Uvinul [®] 3000, 63
213	228	119	91	65	228.29	100	22	16	10	7	Bisphenol A, 253
213	326	43	137	105	326.43	100	37	36	33	32	Uvinul [®] 3008, 65
219	57	232	203	552	552.79	100	88	63	47	46	Irganox [®] MD 1024, 159
219	57	304	203	638	638.92	100	51	42	40	38	Irganox [®] 259, 153
219	191	234	57	220	775.32	100	27	26	18	16	Ethanox [®] 330, 134
219	218	217	108	115	219.28	100	64	51	23	16	Naugard [®] PANA, 189
219	234	220	57	159	234.38	100	23	17	10	5	2,6-Di-tert-butyl-4-ethylphenol, 99
300	315	302	272	301	315.80	100	44	34	21	19	2,6-Di-tert-butyl-4-ethylphenol, 101
219	263	58	163	203	263.42	100	26	19	12	12	Ethanox [®] 703, 141
219	341	356	203	147	356.44	100	83	72	58	56	Diethyl 3,5-Di-tert-butyl-4-hydroxybenzylphosphonate, 125
315	91	316	330	103	356.44	100	46	30	30	27	Diethyl 3,5-Di-tert-butyl-4-hydroxybenzylphosphonate, 125
221	250	222	192	71	250.38	100	19	16	10	8	Lowinox [®] AH25, 167
225	93	65	168	154	225.27	100	20	12	10	18	Tinuvin [®] PED, 71
226	225	165	227	152	N/A	100	45	28	16	10	Vinsol [®] resin, 385
227	151	228	77	51	228.26	100	81	66	38	21	Uvinul [®] 3040, 67
232	301	141	797	959	959.22	100	61	60	22	9	Decabromodiphenyl ether, 238
233	217	204	234	438	438.69	100	40	22	18	14	2,2'-Ethylidene-bis(4,6-di-tert-butylphenol), 145
233	247	234	262	57	N/A	100	28	18	17	15	Naugard [®] PS-35, 199
233	247	262	57	217	262.43	100	29	17	10	6	Isonox [®] 132, 161
233	248	234	205		775.32	100	24	17	16		Ethanox [®] 330, 135
233	304	234	43	107	304.58	100	39	17	16	15	Santoflex [®] 77PD, 57
240	239	165	241	152	N/A	100	45	26	18	13	Vinsol [®] resin, 385
241	185	55	56	57	314.46	100	72	31	29	24	Dibutyl Sebacate, 277
247	57	261	248	332	332.57	100	32	25	19	4	Isonox [®] 232, 164
247	261	57	55	332	332.57	100	64	63	23	5	Isonox [®] 232, 165
251	250	94	249	252	362.40	100	24	18	16	13	Santicizer [®] 141, 372, 373

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252	253	105	323	133	323.43	100	18	7	5	5	2-(2-Hydroxy-5-t-octylphenyl)benzotriazole, 83
260	261	183	167	77	260.36	100	21	17	16	15	Naugard® J, 185
261	149	70	112	167	390.56	100	99	93	82	65	bis(2-Ethylhexyl) terephthalate, 305
266	98	194	123	85	~255	100	31	28	24	19	Halowax 1001, 243
266	267	337	250	322	N/A	100	23	15	10	7	Naugard® PS-30, 196
266	267	337	250	393	N/A	100	21	14	10	1	Naugard® PS-35, 199
266	281	267	97	125	N/A	100	32	21	15	7	Naugard® PS-30, 195
277	57	292	147	219	1177.65	100	41	37	28	23	Naugard® B-25, 179
277	147	292	57	219	460.73	100	44	32	23	10	BNX 1077, 93
277	193	278	379	462	462.62	100	22	17	8	1	Morflex® 560, 351
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